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NEWS 12 MAY 11
                 BEILSTEIN substance information now available on
                 STN Easy
                 DGENE, PCTGEN and USGENE enhanced with increased
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         MAY 14
                 limits for exact sequence match searches and
                 introduction of free HIT display format
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MF C31 H36 N6 O5 S

## HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

- L2 83 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN
- IN 2-Furancarboxylic acid, 5-[3-[[[4-[[4-[[4-(dimethylamino)-1-oxobutyl]amino]-1-methyl-1H-pyrrol-2-yl]carbonyl]amino]-1-methyl-1H-pyrrol-2-yl]carbonyl]amino]phenyl]-, methyl ester
- MF C30 H34 N6 O6

\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

- L2 83 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN
- IN 2-Thiophenecarboxylic acid, 5-[4-[[[4-[[[4-[[[4-[[(1,1-dimethylethoxy)carbonyl]amino]-1-methyl-1H-pyrrol-2-yl]carbonyl]amino]-1-methyl-1H-pyrrol-2-yl]carbonyl]amino]phenyl]-, ethyl ester

## HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

L2 83 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN

IN 4-Thiazolecarboxylic acid, 2-[4-[[[4-[[[4-[[[4-[[(1,1-dimethylethoxy)carbonyl]amino]-1-methyl-1H-pyrrol-2-yl]carbonyl]amino]-1-methyl-1H-pyrrol-2-yl]carbonyl]amino]phenyl]-, ethyl ester

MF C29 H32 N6 O6 S

\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

L2 83 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN

IN 2-Furancarboxamide, 5-(4-aminophenyl)-N-methyl-

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

L2 83 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN

IN 1H-Pyrrole-2-carboxylic acid, 4-(4-aminophenyl)-1-methyl-, methyl ester MF C13 H14 N2 O2

\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

L2 83 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN

IN 2-Thiophenecarboxylic acid, 5-(4-aminophenyl)-, ethyl ester

MF C13 H13 N O2 S

\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

L2 83 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN

IN [1,1'-Biphenyl]-3-carboxylic acid,
 4'-[[4-[[4-[[(1,1-dimethylethoxy)carbonyl]amino]-1-methyl-1H-pyrrol-2 yl]carbonyl]amino]-1-methyl-1H-pyrrol-2-yl]carbonyl]amino]-, methyl ester
MF C31 H33 N5 O6

\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

L2 83 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN

IN 2-Furancarboxamide, 5-(4-aminophenyl)-N,N-dimethyl-

MF C13 H14 N2 O2

CI COM

\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

L2 83 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN

IN Benzenamine, 4-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)-

MF C12 H18 B N O2

CI COM

\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

L2 83 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN

IN 2-Furancarboxamide, 5-(4-aminophenyl)-

MF C11 H10 N2 O2

$$H_2N-C$$
 $NH_2$ 

\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

L2 83 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN

IN 2-Furancarboxylic acid, 5-(3-aminophenyl)-, methyl ester

MF C12 H11 N O3

\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

L2 83 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN

IN 2-Furancarboxylic acid, 5-(4-nitrophenyl)-

MF C11 H7 N O5

\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L2 83 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN

IN Pyridine, 2-bromo-5-nitro-

MF  $C\bar{5}$  H3 Br N2 O2

CI COM

\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

L2 83 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN

IN Benzene, 1-bromo-4-nitro-

MF C6 H4 Br N O2

CI COM

\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

L2 83 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN

IN 1,3-Propanediamine, N1,N1-dimethyl-

MF C5 H14 N2

CI COM

 $H_2N-(CH_2)_3-NMe_2$ 

\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

L2 83 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN

IN 1H-Pyrrolo[2,1-c][1,4]benzodiazepine-10(5H)-carboxylic acid, 8-(3-carboxypropoxy)-2,3,11,11a-tetrahydro-11-hydroxy-7-methoxy-5-oxo-, <math>10-(1,1-dimethylethyl) ester

MF C22 H30 N2 O8

$$t-BuO-C$$
 OH

 $HO_2C-(CH_2)_3-O$ 
 $MeO$ 
 $N$ 
 $N$ 
 $N$ 

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

L2 83 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN

IN 1H-Pyrrole-2-carboxylic acid, 4-[4-[[[4-[[4-[[4-([i4-(imethylamino)-1-oxobutyl]amino]-1-methyl-1H-pyrrol-2-yl]carbonyl]amino]-1-methyl-1H-pyrrol-2-yl]carbonyl]amino]phenyl]-1-methyl-, methyl ester

MF C31 H37 N7 O5

\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

- L2 83 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN
- IN Benzoic acid, 3-[5-[[[4-[[4-(dimethylamino)-1-oxobutyl]amino]-1-methyl-1H-pyrrol-2-yl]carbonyl]amino]-1-methyl-1H-pyrrol-2-yl]carbonyl]amino]-2-pyridinyl]-, methyl ester

MF C31 H35 N7 O5

PAGE 1-A

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PAGE 1-B

- OMe

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HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

- L2 83 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN

\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

L2 83 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN

IN 2-Furancarboxamide, 5-(4-aminophenyl)-N-[3-(dimethylamino)propyl]-MF C16 H21 N3 O2

$$Me_2N-(CH_2)_3-NH-C$$

\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

L2 83 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN

\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

L2 83 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN

IN 1H-Pyrrole-2-carboxylic acid, 4-[4-[[(1,1-

dimethylethoxy)carbonyl]amino]phenyl]-1-methyl-, methyl ester

MF C18 H22 N2 O4

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

L2 83 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN

IN Benzoic acid, 3-(5-amino-2-pyridinyl)-, methyl ester

MF C13 H12 N2 O2

\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

L2 83 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN

IN 2-Furancarboxylic acid, 5-[4-[[(1,1-dimethylethoxy)carbonyl]amino]phenyl]-

MF C16 H17 N O5

\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L2 83 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN

IN 4-Thiazolecarboxylic acid, 2-[4-[[(1,1-

dimethylethoxy)carbonyl]amino]phenyl]-

MF C15 H16 N2 O4 S

\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

L2 83 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN

IN 1H-Pyrrole-2-carboxylic acid, 4-[[[4-[[(1,1-dimethylethoxy)carbonyl]amino]-1-methyl-1H-pyrrol-2-yl]carbonyl]amino]-1-methyl-

MF C17 H22 N4 O5

\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

L2 83 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN

IN 1H-Pyrrole-2-carboxylic acid, 4-[[(1,1-dimethylethoxy)carbonyl]amino]-1methyl-

MF C11 H16 N2 O4

CI COM

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

L2 83 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN

IN 2-Furancarboxylic acid, 5-(4-nitrophenyl)-, methyl ester

MF C12 H9 N O5

\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

L2 83 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN

IN Benzoic acid, 3-borono-

MF C7 H7 B O4

\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

L2 83 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN

IN [1,1'-Biphenyl]-3-carboxylic acid, 4'-nitro-

MF C13 H9 N O4

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

L2 83 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN

IN Morpholine

MF C4 H9 N O

CI COM, RPS

\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

L2 83 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN

IN Acetyl chloride, 2,2,2-trichloro-

MF C2 C14 O

CI COM

\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

- L2 83 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN
- IN 1H-Pyrrolo[2,1-c][1,4]benzodiazepine-10(5H)-carboxylic acid,
  2,3,11,11a-tetrahydro-11-hydroxy-7-methoxy-8-[4-[[3-[5-(methoxycarbonyl)-2-furanyl]phenyl]amino]-4-oxobutoxy]-5-oxo-, 1,1-dimethylethyl ester
  MF C34 H39 N3 O10

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

L2 83 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN

IN 4-Thiazolecarboxylic acid, 2-[4-[[[4-[[4-[[4-(dimethylamino)-1-oxobutyl]amino]-1-methyl-1H-pyrrol-2-yl]carbonyl]amino]-1-methyl-1H-pyrrol-2-yl]carbonyl]amino]phenyl]-, ethyl ester

MF C30 H35 N7 O5 S

\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

- L2 83 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN
- IN 1H-Imidazole-2-carboxylic acid, 4-[4-[[4-[[4-[[4-[[4-[[(1,1-dimethylethoxy)carbonyl]amino]-1-methyl-1H-pyrrol-2-yl]carbonyl]amino]-1-methyl-1H-pyrrol-2-yl]carbonyl]amino]phenyl]-1-methyl-, methyl ester

MF C29 H33 N7 O6

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

L2 83 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN

\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

L2 83 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN

IN Methanone, [5-(4-aminophenyl)-2-furanyl]-4-morpholinyl-

MF C15 H16 N2 O3

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

L2 83 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN

IN 1H-Imidazole-2-carboxylic acid, 4-bromo-1-methyl-, methyl ester

MF C6 H7 Br N2 O2

\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

L2 83 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN

IN 4-Thiazolecarboxylic acid, 2-[4-[[4-[4-(dimethylamino)-1-oxobutyl]amino]-1-oxobutyl]

1-methyl-1H-pyrrol-2-yl]carbonyl]amino]phenyl]-, ethyl ester

MF C24 H29 N5 O4 S

\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

L2 83 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN

IN Benzoic acid, 3-(5-nitro-2-pyridinyl)-

MF C12 H8 N2 O4

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

L2 83 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN

MF C27 H26 N4 O5 S2

\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

L2 83 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN

IN Carbamic acid, N-[4-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)phenyl]-, 1,1-dimethylethyl ester

MF C17 H26 B N O4

\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L2 83 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN

[1,1'-Biphenyl]-3-carboxylic acid, 4'-nitro-, methyl ester

MF C14 H11 N O4

ΙN

\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

L2 83 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN

IN 2-Thiophenecarboxylic acid, 5-bromo-, methyl ester

MF C6 H5 Br O2 S

\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

L2 83 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN

IN Ethanone, 2,2,2-trichloro-1-(1-methyl-1H-imidazol-2-yl)-

MF C6 H5 C13 N2 O

\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L2 83 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN

IN 2-Furancarboxylic acid, 5-(3-nitrophenyl)-

MF C11 H7 N O5

\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

L2 83 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN

IN Benzamide, 4-nitro-

MF C7 H6 N2 O3

CI COM

$$\begin{array}{c|c} \circ \\ \parallel \\ C-\mathrm{NH_2} \end{array}$$

\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

L2 83 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN

IN Ethanamine, N-ethyl-

MF C4 H11 N

CI COM

H<sub>3</sub>C-CH<sub>2</sub>-NH-CH<sub>2</sub>-CH<sub>3</sub>

\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

L2 83 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN

IN 5-Thiazolecarboxylic acid, 2-[4-[[(1,1-

dimethylethoxy)carbonyl]amino]phenyl]-4-methyl-

MF C16 H18 N2 O4 S

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

L2 83 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN

IN 1H-Imidazole-2-carboxylic acid, 4-[4-[[4-[[4-[[4-(dimethylamino)-1-oxobutyl]amino]-1-methyl-1H-pyrrol-2-yl]carbonyl]amino]-1-methyl-1H-pyrrol-2-yl]carbonyl]amino]phenyl]-1-methyl-, methyl ester

MF C30 H36 N8 O5

\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

- L2 83 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN
- IN 2-Furancarboxylic acid, 5-[4-[[4-[[4-[[4-(dimethylamino)-1-oxobutyl]amino]-1-methyl-1H-pyrrol-2-yl]carbonyl]amino]-1-methyl-1H-pyrrol-2-yl]carbonyl]amino]phenyl]-, methyl ester

MF C30 H34 N6 O6

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

- L2 83 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN
- IN 1H-Pyrrole-2-carboxylic acid, 4-[4-[[[4-[[[4-[[[4-[[[4-[[[4-[[[4-[[1]]
  dimethylethoxy)carbonyl]amino]-1-methyl-1H-pyrrol-2-yl]carbonyl]amino]-1methyl-1H-pyrrol-2-yl]carbonyl]amino]phenyl]-1-methyl-, methyl ester
- MF C30 H34 N6 O6

\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

- L2 83 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN
- IN 2-Furancarboxamide, N, N'-1, 4-butanediylbis[5-(4-aminophenyl)-

$$^{\rm NH}_{2}$$
N  $^{\rm O}$   $^{\rm O}$   $^{\rm C}$   $^{\rm NH}_{2}$   $^{\rm O}$   $^{\rm O}$   $^{\rm O}$   $^{\rm NH}_{2}$ 

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

L2 83 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN

IN 1H-Imidazole-2-carboxylic acid, 4-[4-[[(1,1dimethylethoxy)carbonyl]amino]phenyl]-1-methyl-

MF C16 H19 N3 O4

MF

\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

L2 83 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN

IN 1H-Pyrrole-2-carboxylic acid, 4-[4-[[(1,1-

dimethylethoxy)carbonyl]amino]phenyl]-1-methyl-C17 H20 N2 O4

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

L2 83 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN

IN 2-Furancarboxylic acid, 5-[3-[[(1,1-dimethylethoxy)carbonyl]amino]phenyl]-

MF C16 H17 N O5

\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

- L2 83 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN

MF C29 H31 N5 O7

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

L2 83 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN

IN 4-Thiazolecarboxylic acid, 2-(4-aminophenyl)-, ethyl ester

MF C12 H12 N2 O2 S

CI COM

\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

L2 83 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN

IN Ethanone, 1-(4-bromo-1-methyl-1H-pyrrol-2-yl)-2,2,2-trichloro-

MF C7 H5 Br C13 N O

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

L2 83 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN

IN 4-Thiazolecarboxylic acid, 2-(4-nitrophenyl)-, ethyl ester

MF C12 H10 N2 O4 S

\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

L2 83 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN

IN 2-Furancarboxylic acid, 5-(4-aminophenyl)-, methyl ester

MF C12 H11 N O3

CI COM

$$\begin{array}{c} O \\ || \\ || \\ O \\ NH_2 \end{array}$$

\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

L2 83 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN

IN Benzenecarbothioamide, 4-nitro-

MF C7 H6 N2 O2 S

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

L2 83 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN

IN 1H-Pyrrole-2-carboxylic acid, 4-bromo-1-methyl-, methyl ester

MF C7 H8 Br N O2

\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

L2 83 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN

IN 4-Morpholinepropanamine

MF C7 H16 N2 O

CI COM

\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

L2 83 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN

IN 1H-Pyrrole, 1-methyl-

MF C5 H7 N

CI COM

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

L2 83 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN

IN 2-Furancarboxylic acid, 5-[3-[[1-oxo-4-[(2,3,5,11a-tetrahydro-7-methoxy-5oxo-1H-pyrrolo[2,1-c][1,4]benzodiazepin-8-yl)oxy]butyl]amino]phenyl]-,
methyl ester

MF C29 H29 N3 O7

$$MeO-C \longrightarrow 0 \longrightarrow NH-C-(CH_2)_3-0 \longrightarrow NH-C-(CH_2)_3-0$$

\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

- L2 83 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN
- IN 5-Thiazolecarboxylic acid, 2-[4-[[[4-[[4-[[4-(dimethylamino)-1-oxobutyl]amino]-1-methyl-1H-pyrrol-2-yl]carbonyl]amino]-1-methyl-1H-pyrrol-2-yl]carbonyl]amino]phenyl]-4-methyl-, ethyl ester
- MF C31 H37 N7 O5 S

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

L2 83 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN

IN [1,1'-Biphenyl]-3-carboxylic acid,

4'-[[[4-[[4-[[4-(dimethylamino)-1-oxobutyl]amino]-1-methyl-1H-pyrrol-2-yl]carbonyl]amino]-1-methyl-1H-pyrrol-2-yl]carbonyl]amino]-, methyl ester

MF C32 H36 N6 O5

PAGE 1-A

PAGE 1-B

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

L2 83 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN

\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

L2 83 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN

IN 2-Furancarboxamide, 5-(4-aminophenyl)-N-[3-(4-morpholinyl)propyl]-

MF C18 H23 N3 O3

\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

L2 83 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN

IN 1H-Imidazole-2-carboxylic acid, 4-(4-aminophenyl)-1-methyl-, methyl ester

MF C12 H13 N3 O2

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

L2 83 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN

IN 4-Thiazolecarboxylic acid, 2-[4-[[[4-[[(1,1-dimethylethoxy)carbonyl]amino]-1-methyl-1H-pyrrol-2-yl]carbonyl]amino]phenyl]-, ethyl ester

MF C23 H26 N4 O5 S

\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

L2 83 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN

IN Benzoic acid, 3-(5-nitro-2-pyridinyl)-, methyl ester

MF C13 H10 N2 O4

\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

L2 83 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN

\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

L2 83 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN IN [1,1'-Biphenyl]-3-carboxylic acid, 4'-amino-, methyl ester

MF C14 H13 N O2

\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

L2 83 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN

IN 1H-Pyrrole-2-carboxylic acid, 4-[[[4-[[(1,1-dimethylethoxy)carbonyl]amino]-1-methyl-1H-pyrrol-2-yl]carbonyl]amino]-1-methyl-, methyl ester

MF C18 H24 N4 O5

\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

# HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

L2 83 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN

IN 5-Thiazolecarboxylic acid, 2-(4-aminophenyl)-4-methyl-, ethyl ester

MF C13 H14 N2 O2 S

CI COM

\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

L2 83 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN

IN 2-Furancarboxylic acid, 5-(3-nitrophenyl)-, methyl ester

MF C12 H9 N O5

$$MeO-C \longrightarrow 0 \longrightarrow NO_2$$

\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

L2 83 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN

IN Ethanone, 2,2,2-trichloro-1-(1-methyl-1H-pyrrol-2-yl)-

MF C7 H6 C13 N O

\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

L2 83 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN

IN Butanoic acid, 4-(dimethylamino)-

MF C6 H13 N O2

CI COM

 $Me_2N - (CH_2)_3 - CO_2H$ 

\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

L2 83 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN

IN 1,4-Butanediamine

MF C4 H12 N2

CI COM

 $H_2N^-$  (CH<sub>2</sub>)<sub>4</sub> $-NH_2$ 

\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

L2 83 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN

IN Propanoic acid, 3-bromo-2-oxo-, ethyl ester

MF C5 H7 Br O3

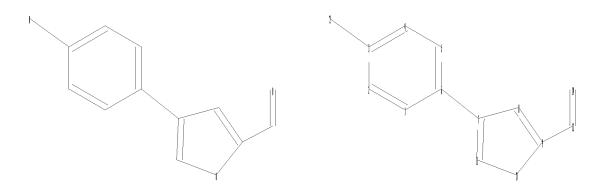
$$\begin{array}{c|c} & \text{O} & \text{O} \\ & || & || \\ \text{BrCH}_2 - \text{C} - \text{C} - \text{OEt} \end{array}$$

\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

ALL ANSWERS HAVE BEEN SCANNED

=>

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chain nodes :
12 13 14
ring nodes :
1 2 3 4 5 6 7 8 9 10 11
chain bonds :
3-12 6-7 9-13 13-14
ring bonds :
1-2 1-6 2-3 3-4 4-5 5-6 7-8 7-11 8-9 9-10 10-11
exact/norm bonds :
3-12 9-10 10-11 13-14
exact bonds :
6-7 7-8 7-11 8-9 9-13
normalized bonds :
1-2 1-6 2-3 3-4 4-5 5-6
isolated ring systems :

Match level :

containing 1 : 7 :

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom 11:Atom 12:CLASS 13:CLASS 14:CLASS

# L3 STRUCTURE UPLOADED

=> s sam sss 13 SAMPLE SEARCH INITIATED 15:55:51 FILE 'REGISTRY' SAMPLE SCREEN SEARCH COMPLETED - 252 TO ITERATE

100.0% PROCESSED 252 ITERATIONS 7 ANSWERS

SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE \*\*COMPLETE\*\*
BATCH \*\*COMPLETE\*\*
PROJECTED ITERATIONS: 4088 TO 5992
PROJECTED ANSWERS: 7 TO 298

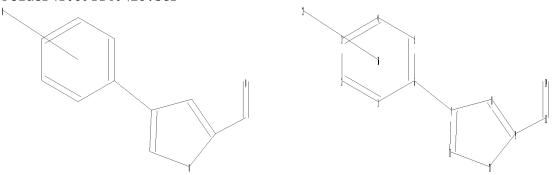
L4 7 SEA SSS SAM L3

=> d sca

L4 7 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN
IN 1H-Pyrrole-2-carboxylic acid, 5-nitro-4-(4-nitrophenyl)-, ethyl ester
MF C13 H11 N3 O6

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):0

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chain nodes : 12 13 14 ring nodes : 1 2 3 4 5 6 7 8 9 10 11 chain bonds : 6-7 9-13 13-14 ring bonds : 1-2 1-6 2-3 3-4 4-5 5-6 7-8 7-11 8-9 9-10 10-11exact/norm bonds : 9-10 10-11 13-14 exact bonds : 6-7 7-8 7-11 8-9 9-13 normalized bonds : 1-2 1-6 2-3 3-4 4-5 5-6 isolated ring systems : containing 1 : 7 :

Match level:

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom 11:Atom 12:CLASS 13:CLASS 14:CLASS 16:Atom

=> s sam sss 15 SAMPLE SEARCH INITIATED 15:58:10 FILE 'REGISTRY' SAMPLE SCREEN SEARCH COMPLETED - 1512 TO ITERATE

100.0% PROCESSED 1512 ITERATIONS 11 ANSWERS

SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE \*\*COMPLETE\*\*
BATCH \*\*COMPLETE\*\*
PROJECTED ITERATIONS: 27908 TO 32572
PROJECTED ANSWERS: 22 TO 418

L6 11 SEA SSS SAM L5

=> d sca

L6 11 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN

IN 1H-Pyrrole-2-carboxamide, 4-[4-[[[[4-(1-

methylethyl)phenyl]amino]carbonyl]amino]phenyl]-N-[2-(4-morpholinyl)ethyl]-

MF C27 H33 N5 O3

\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

L6 11 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN

IN 1H-Pyrrole-2-carboxylic acid, 4-(4-aminophenyl)-1-[(2-chlorophenyl)methyl]-, methyl ester

MF C19 H17 C1 N2 O2

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

L6 11 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN

IN 1H-Pyrrole-2-carboxylic acid, 4-(3-chloro-2-nitrophenyl)-, methyl ester

MF C12 H9 C1 N2 O4

$$\begin{array}{c|c} O & H \\ MeO-C & N \\ \hline \end{array}$$

\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

L6 11 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN

IN 1H-Pyrrole-2-carboxylic acid, 4-(4-aminophenyl)-1-methyl-, methyl ester

MF C13 H14 N2 O2

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

L6 11 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN

IN 1H-Pyrrole-2-carboxylic acid, 4-(4-aminophenyl)-1-hexyl-, methyl ester

MF C18 H24 N2 O2

MF

\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

L6 11 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN

IN 1H-Pyrrole-2-carboxylic acid, 3-chloro-4-(3-chloro-2-nitrophenyl)-5-(dichloromethyl)-, methyl ester

C13 H8 C14 N2 O4

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

L6 11 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN

IN 1H-Pyrrole-2-carboxylic acid, 5-nitro-4-(4-nitrophenyl)-, ethyl ester

MF C13 H11 N3 O6

\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

L6 11 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN

IN 1H-Pyrrole-2-carboxylic acid, 1-[(2-chlorophenyl)methyl]-4-[4-[[(3,5-difluorophenyl)methyl]amino]phenyl]-, methyl ester

MF C26 H21 C1 F2 N2 O2

PAGE 2-A

\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

L6

11 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN 1H-Pyrrole-2-butanoic acid, 5-(methoxycarbonyl)-1,4-dimethyl-3-(2-IN nitrophenyl)-, ethyl ester C20 H24 N2 O6

MF

Me O C N (CH<sub>2</sub>) 
$$_3$$
 C OEt

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

L6 11 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN

IN 1H-Pyrrole-2-carboxylic acid, 4-[4-[[(2,6-

dichlorophenyl)methyl]amino]phenyl]-1-octyl-

MF C26 H30 C12 N2 O2

# \*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

L6 11 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN

IN 1H-Pyrrole-2-carboxylic acid, 3-chloro-4-(3-chloro-2-nitrophenyl)-5-formyl-

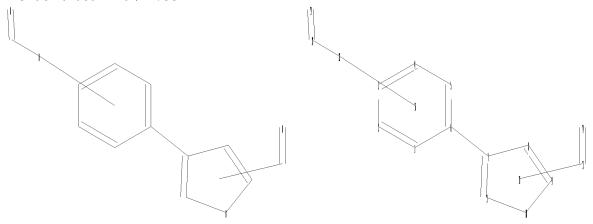
, methyl ester

MF C13 H8 C12 N2 O5

\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

ALL ANSWERS HAVE BEEN SCANNED

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chain nodes:
12 13 14 18 19
ring nodes:

1 2 3 4 5 6 7 8 9 10 11

chain bonds :

6-7 12-18 13-14 18-19

ring bonds :

 $1-2 \quad 1-6 \quad 2-3 \quad 3-4 \quad 4-5 \quad 5-6 \quad 7-8 \quad 7-11 \quad 8-9 \quad 9-10 \quad 10-11$ 

exact/norm bonds :

8-9 9-10 10-11 12-18 13-14 18-19

exact bonds :

6 - 7

normalized bonds :

1-2 1-6 2-3 3-4 4-5 5-6 7-8 7-11

isolated ring systems :

containing 1: 7:

### Match level:

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom 11:Atom 12:CLASS 13:CLASS 14:CLASS 16:Atom 17:Atom 18:CLASS 19:CLASS

### L7 STRUCTURE UPLOADED

=> s sam sss 17

SAMPLE SEARCH INITIATED 16:06:20 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED - 846 TO ITERATE

100.0% PROCESSED 846 ITERATIONS

IONS

0 ANSWERS

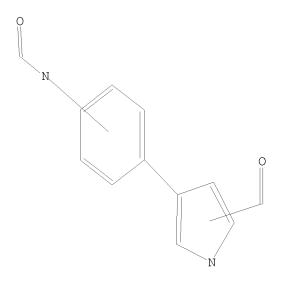
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE \*\*COMPLETE\*\*
BATCH \*\*COMPLETE\*\*

PROJECTED ITERATIONS: 15175 TO 18665
PROJECTED ANSWERS: 0 TO 0

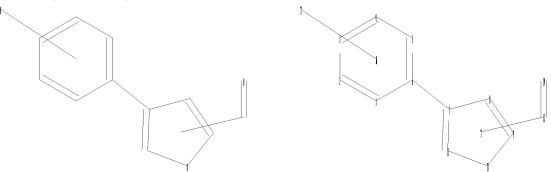
L8 0 SEA SSS SAM L7

=> d 17 L7 HAS NO ANSWERS L7 STR



Structure attributes must be viewed using STN Express query preparation.

=> Uploading C:\Documents and Settings\vrodriguezgarcia\My Documents\e-Red Folder\10591140\L9.str



chain nodes :
12 13 14
ring nodes :
1 2 3 4 5 6 7 8 9 10 11
chain bonds :
6-7 13-14
ring bonds :
1-2 1-6 2-3 3-4 4-5 5-6 7-8 7-11 8-9 9-10 10-11
exact/norm bonds :
8-9 9-10 10-11 13-14
exact bonds :
6-7
normalized bonds :
1-2 1-6 2-3 3-4 4-5 5-6 7-8 7-11
isolated ring systems :
containing 1 : 7 :

Match level:

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom 11:Atom 12:CLASS 13:CLASS 14:CLASS 16:Atom 17:Atom

#### L9 STRUCTURE UPLOADED

=> s sam sss 19 SAMPLE SEARCH INITIATED 16:07:26 FILE 'REGISTRY' SAMPLE SCREEN SEARCH COMPLETED - 3767 TO ITERATE

53.1% PROCESSED 2000 ITERATIONS INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED)

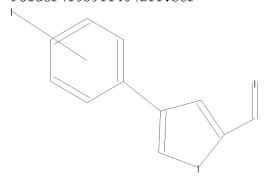
SEARCH TIME: 00.00.01

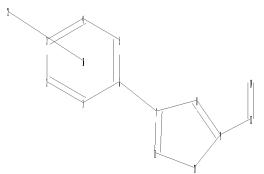
FULL FILE PROJECTIONS: ONLINE \*\*COMPLETE\*\* BATCH \*\*COMPLETE\*\*

PROJECTED ITERATIONS: 71659 TO 79021 PROJECTED ANSWERS: 0 TO

L10 0 SEA SSS SAM L9

Uploading C:\Documents and Settings\vrodriguezgarcia\My Documents\e-Red Folder\10591140\L11.str





0 ANSWERS

chain nodes : 12 13 14 ring nodes : 1 2 3 4 5 6 7 8 9 10 11 chain bonds : 6-7 9-13 13-14 ring bonds : 1-2 1-6 2-3 3-4 4-5 5-6 7-8 7-11 8-9 9-10 10-11exact/norm bonds : 9-10 10-11 13-14

exact bonds : 6-7 7-8 7-11 8-9 9-13 normalized bonds : 1-2 1-6 2-3 3-4 4-5 5-6 isolated ring systems :

Match level:

containing 1 : 7 :

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom 11:Atom 12:CLASS 13:CLASS 14:CLASS 16:Atom

### L11 STRUCTURE UPLOADED

=> s sam sss 111 SAMPLE SEARCH INITIATED 16:08:20 FILE 'REGISTRY' SAMPLE SCREEN SEARCH COMPLETED - 1512 TO ITERATE

100.0% PROCESSED 1512 ITERATIONS 11 ANSWERS

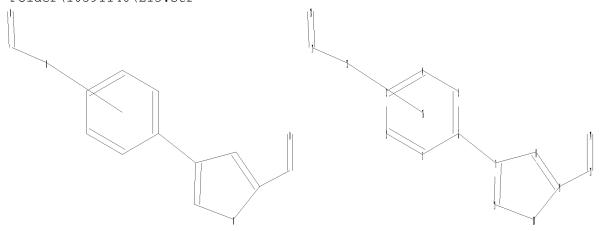
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE \*\*COMPLETE\*\*
BATCH \*\*COMPLETE\*\*
PROJECTED ITERATIONS: 27908 TO 32572
PROJECTED ANSWERS: 22 TO 418

L12 11 SEA SSS SAM L11

=>

Uploading C:\Documents and Settings\vrodriguezgarcia\My Documents\e-Red Folder\10591140\L13.str



chain nodes : 12 13 14 17 18 ring nodes : 1 2 3 4 5 6 7 8 9 10 11 chain bonds : 6-7 9-13 12-17 13-14 17-18 ring bonds :  $1-2 \quad 1-6 \quad 2-3 \quad 3-4 \quad 4-5 \quad 5-6 \quad 7-8 \quad 7-11 \quad 8-9 \quad 9-10 \quad 10-11$ exact/norm bonds : 9-10 10-11 12-17 13-14 17-18 exact bonds : 6-7 7-8 7-11 8-9 9-13 normalized bonds : 1-2 1-6 2-3 3-4 4-5 5-6 isolated ring systems : containing 1 : 7 :

Match level:

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom 11:Atom 12:CLASS 13:CLASS 14:CLASS 16:Atom 17:CLASS 18:CLASS

## L13 STRUCTURE UPLOADED

 $\Rightarrow$  s sam sss 113

SAMPLE SEARCH INITIATED 16:09:20 FILE 'REGISTRY'

SAMPLE SCREEN SEARCH COMPLETED - 1512 TO ITERATE

100.0% PROCESSED 1512 ITERATIONS

1 ANSWERS

SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE \*\*COMPLETE\*\*

BATCH \*\*COMPLETE\*\*

PROJECTED ITERATIONS: 27908 TO 32572 PROJECTED ANSWERS: 1 TO 80

L14 1 SEA SSS SAM L13

=> d sca

L14 1 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN

IN 1H-Pyrrole-2-carboxamide, 4-[4-[[[4-(1-

methylethyl)phenyl]amino]carbonyl]amino]phenyl]-N-[2-(4-morpholinyl)ethyl]-

MF C27 H33 N5 O3

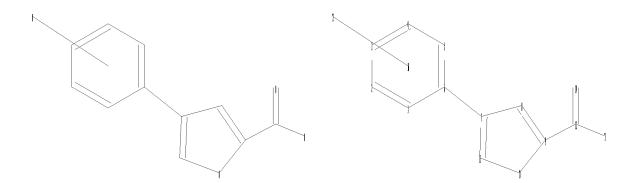
$$\begin{array}{c|c} & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ &$$

\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

ALL ANSWERS HAVE BEEN SCANNED

=>

Uploading C:\Documents and Settings\vrodriguezgarcia\My Documents\e-Red Folder\10591140\L15.str



chain nodes :
12 13 14 17
ring nodes :
1 2 3 4 5 6 7 8 9 10 11
chain bonds :
6-7 9-13 13-14 13-17
ring bonds :
1-2 1-6 2-3 3-4 4-5 5-6 7-8 7-11 8-9 9-10 10-11
exact/norm bonds :
9-10 10-11 13-14 13-17
exact bonds :
6-7 7-8 7-11 8-9 9-13
normalized bonds :
1-2 1-6 2-3 3-4 4-5 5-6
isolated ring systems :

Match level :

containing 1 : 7 :

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom 11:Atom 12:CLASS 13:CLASS 14:CLASS 16:Atom 17:CLASS

## L15 STRUCTURE UPLOADED

=> s sam sss 115 SAMPLE SEARCH INITIATED 16:11:17 FILE 'REGISTRY' SAMPLE SCREEN SEARCH COMPLETED - 816 TO ITERATE

100.0% PROCESSED 816 ITERATIONS 1 ANSWERS

SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE \*\*COMPLETE\*\*
BATCH \*\*COMPLETE\*\*
PROJECTED ITERATIONS: 14607 TO 18033
PROJECTED ANSWERS: 1 TO 80

L16 1 SEA SSS SAM L15

=> d sca

ALL ANSWERS HAVE BEEN SCANNED

=> => file zcaplus COST IN U.S. DOLLARS

FULL ESTIMATED COST

SINCE FILE TOTAL ENTRY SESSION 16.32 23.90

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FILE COVERS 1907 - 17 Jun 2009 VOL 150 ISS 25
FILE LAST UPDATED: 16 Jun 2009 (20090616/ED)
REVISED CLASS FIELDS (/NCL) LAST RELOADED: Apr 2009
USPTO MANUAL OF CLASSIFICATIONS THESAURUS ISSUE DATE: Feb 2009

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This file contains CAS Registry Numbers for easy and accurate substance identification.

=> s polyamide

149272 POLYAMIDE

129830 POLYAMIDES

L17 199018 POLYAMIDE

(POLYAMIDE OR POLYAMIDES)

=> file registry

COST IN U.S. DOLLARS

SINCE FILE TOTAL ENTRY SESSION

26.80

2.90

FULL ESTIMATED COST

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STRUCTURE FILE UPDATES: 15 JUN 2009 HIGHEST RN 1158168-92-3 DICTIONARY FILE UPDATES: 15 JUN 2009 HIGHEST RN 1158168-92-3

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=> s full 111

THE ESTIMATED SEARCH COST FOR FILE 'REGISTRY' IS 185.40 U.S. DOLLARS DO YOU WANT TO CONTINUE WITH THIS REQUEST? (Y)/N or END:n SEARCH ENDED BY USER

=> s full sss 111

THE ESTIMATED SEARCH COST FOR FILE 'REGISTRY' IS 185.40 U.S. DOLLARS DO YOU WANT TO CONTINUE WITH THIS REQUEST? (Y)/N or END:y FULL SEARCH INITIATED 16:38:37 FILE 'REGISTRY' FULL SCREEN SEARCH COMPLETED - 29741 TO ITERATE

100.0% PROCESSED 29741 ITERATIONS SEARCH TIME: 00.00.02

185 ANSWERS

L18 185 SEA SSS FUL L11

=> d sca

L18 185 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN

\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

L18 185 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN IN 1H-Pyrrole-2-butanoic acid, 1,3-dimethyl-4-(2-nitrophenyl)- $\gamma$ -oxo-, ethyl ester MF C18 H20 N2 O5

\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

L18 185 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN
IN 1H-Pyrrole-2-carboxaldehyde, 3-chloro-4-(3-chloro-2-nitrophenyl)MF C11 H6 C12 N2 O3

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

L18 185 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN

IN 1H-Pyrrole-2-carboxylic acid, 1-[(6-chloro-1,3-benzodioxol-5-yl)methyl]-4-(4-nitrophenyl)-, methyl ester

MF C20 H15 C1 N2 O6

$$\begin{array}{c} O \\ C-OMe \\ \end{array}$$

\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

L18 185 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN

IN 1H-Pyrrole-3-butanoic acid, 2-(ethoxycarbonyl)-1-methyl-4-(2-nitrophenyl)-  $\gamma$ -oxo-, ethyl ester

MF C20 H22 N2 O7

\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):0

=> file zcaplus

COST IN U.S. DOLLARS SINCE FILE TOTAL ENTRY SESSION 206.04 232.84

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FILE COVERS 1907 - 17 Jun 2009 VOL 150 ISS 25 FILE LAST UPDATED: 16 Jun 2009 (20090616/ED) REVISED CLASS FIELDS (/NCL) LAST RELOADED: Apr 2009 USPTO MANUAL OF CLASSIFICATIONS THESAURUS ISSUE DATE: Feb 2009

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=> s 118

L19 64 L18

=> s 119 and (polyamide or polyamido)

149272 POLYAMIDE 129830 POLYAMIDES

199018 POLYAMIDE

99018 POLIAMIDE

(POLYAMIDE OR POLYAMIDES)

395 POLYAMIDO

L20 0 L19 AND (POLYAMIDE OR POLYAMIDO)

=> s 119 (w) (polyamide or polyamido)

149272 POLYAMIDE

129830 POLYAMIDES

199018 POLYAMIDE

(POLYAMIDE OR POLYAMIDES)

395 POLYAMIDO

L21 0 L19 (W) (POLYAMIDE OR POLYAMIDO)

=> file registry

COST IN U.S. DOLLARS SINCE FILE TOTAL ENTRY SESSION

FULL ESTIMATED COST 11.60 244.44

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TSCA INFORMATION NOW CURRENT THROUGH January 9, 2009.

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http://www.cas.org/support/stngen/stndoc/properties.html

=> s 118 sub=L14 sam
SAMPLE SUBSET SEARCH INITIATED 16:44:02 FILE 'REGISTRY'
SAMPLE SUBSET SCREEN SEARCH COMPLETED - 1 TO ITERATE

100.0% PROCESSED 1 ITERATIONS 1 ANSWERS SEARCH TIME: 00.00.01

PROJECTIONS (WITHIN SPECIFIED SUBSET): ONLINE \*\*COMPLETE\*\*
PROJECTED ITERATIONS (WITHIN SPECIFIED SUBSET): 1 TO 80
PROJECTED ANSWERS (WITHIN SPECIFIED SUBSET): 1 TO 80

L22 1 SEA SUB=L14 SSS SAM L11

=> d sca

MF

L22 1 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN

1H-Pyrrole-2-carboxamide, 4-[4-[[[[4-(1-methylethyl)phenyl]amino]carbonyl]amino]phenyl]-N-[2-(4-morpholinyl)ethyl]-C27 H33 N5 O3

### ALL ANSWERS HAVE BEEN SCANNED

=> s 114 full sub=L18
THE ESTIMATED SEARCH COST FOR FILE 'REGISTRY' IS 44.00 U.S. DOLLARS
DO YOU WANT TO CONTINUE WITH THIS REQUEST? (Y)/N or END:y
FULL SUBSET SEARCH INITIATED 16:46:01 FILE 'REGISTRY'
FULL SUBSET SCREEN SEARCH COMPLETED - 185 TO ITERATE

100.0% PROCESSED 185 ITERATIONS 16 ANSWERS

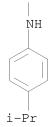
SEARCH TIME: 00.00.01

L23 16 SEA SUB=L18 SSS FUL L13

=> d sca

L23 16 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN
IN 1H-Pyrrole-2-carboxylic acid, 4-[4-[[[4-(1 methylethyl)phenyl]amino]carbonyl]amino]phenyl]-1-[(4 methylphenyl)sulfonyl]-, phenylmethyl ester
MF C35 H33 N3 O5 S

PAGE 2-A



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

L23 16 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN

IN 1H-Pyrrole-2-carboxylic acid, 4-[3-[[([1,1'-biphenyl]-4 ylamino)carbonyl]amino]phenyl]-1-[(4-methylphenyl)sulfonyl]-, phenylmethyl
 ester

MF C38 H31 N3 O5 S

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

L23 16 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN
IN 1H-Pyrrole-2-carboxylic acid, 4-[4-[[(1,1-dimethylethoxy)carbonyl]amino]phenyl]-1-methylMF C17 H20 N2 O4

\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

L23 16 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN

IN 1H-Pyrrole-2-carboxylic acid, 4-[4-[[(1,1-dimethylethoxy)carbonyl]amino]phenyl]-1-(2-nitrophenyl)-, methyl ester

MF C23 H23 N3 O6

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

L23 16 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN

IN Acetamide, N-[3-[5-formyl-1-[(4-methylphenyl)sulfonyl]-1H-pyrrol-3-yl]phenyl]-

MF C20 H18 N2 O4 S

\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

L23 16 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN
IN 1H-Pyrrole-2-carboxylic acid, 3,5-dimethyl-4-[3-[[4-(trifluoromethyl)benzoyl]amino]phenyl]-, ethyl ester
MF C23 H21 F3 N2 O3

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

L23 16 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN

\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

L23 16 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN

MF C18 H22 N2 O4

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

L23 16 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN

IN 1H-Pyrrole-2-carboxylic acid, 4-[4-[[4-[[4-[[4-(dimethylamino)-1-oxobutyl]amino]-1-methyl-1H-pyrrol-2-yl]carbonyl]amino]-1-methyl-1H-pyrrol-2-yl]carbonyl]amino]phenyl]-1-methyl-, methyl ester

MF C31 H37 N7 O5

\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

L23 16 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN

IN 1H-Pyrrole-2-carboxylic acid, 4-[5-[[[1-(2,2-difluoro-1,3-benzodioxol-5-y1)cyclopropyl]carbonyl]amino]-2-methylphenyl]-

MF C23 H18 F2 N2 O5

$$\begin{array}{c|c} & & & & \\ & & \\ & & & \\ & & & \\ & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\$$

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

L23 16 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN

IN 1H-Pyrrole-2-carboxylic acid, 5-(1-cyano-1-ethylpropyl)-4-[2-[[(1,1-dimethylethoxy)carbonyl]amino]phenyl]-1-methyl-, methyl ester
MF C24 H31 N3 O4

\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

L23 16 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):0

=> file zcaplus
COST IN U.S. DOLLARS

SINCE FILE TOTAL ENTRY SESSION 47.36 291.80

FULL ESTIMATED COST

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This file contains CAS Registry Numbers for easy and accurate substance identification.

=> s 123

L24

8 L23

=> s 124 and polyamid3

3 IS NOT A RECOGNIZED COMMAND

The previous command name entered was not recognized by the system. For a list of commands available to you in the current file, enter "HELP COMMANDS" at an arrow prompt (=>).

=> s 124 and polyamid3

3 IS NOT A RECOGNIZED COMMAND

The previous command name entered was not recognized by the system. For a list of commands available to you in the current file, enter "HELP COMMANDS" at an arrow prompt (=>).

=> s 124 and polyamid3

3 IS NOT A RECOGNIZED COMMAND

The previous command name entered was not recognized by the system. For a list of commands available to you in the current file, enter "HELP COMMANDS" at an arrow prompt (=>).

=> s 124 and polyamid#3

'#' TRUNCATION SYMBOL NOT VALID WITHIN 'POLYAMID#3'

The truncation symbol # may be used only at the end of a search term. To specify a variable character within a word use '!', e.g., 'wom!n' to search for both 'woman' and 'women'. Enter "HELP TRUNCATION" at an arrow prompt (=>) for more information.

L25 0 L24 AND ?POLYAMID?

=> d ibib hitstr 1-8

L25 HAS NO ANSWERS

'IBIB HITSTR ' IS NOT A VALID STRUCTURE FORMAT KEYWORD

Structure Formats

SIA ---- Structure Image, Attributes, and map table if it contains data. (Default)

SIM ---- Structure IMage.

SAT ---- Structure ATtributes and map table if it contains data.

SCT ---- Structure Connection Table and map table if it contains

SDA ---- All Structure DAta (image, attributes, connection table and map table if it contains data).

NOS ---- NO Structure data.

ENTER STRUCTURE FORMAT (SIA), SCT, SDA, SIM, SAT, NOS:cia

'CIA' IS NOT A VALID STRUCTURE FORMAT KEYWORD

Structure Formats

SIA ---- Structure Image, Attributes, and map table if it contains data. (Default)

SIM ---- Structure IMage.

SAT ---- Structure ATtributes and map table if it contains data.

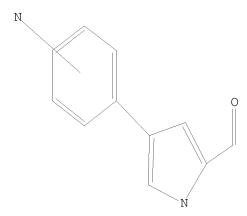
SCT ---- Structure Connection Table and map table if it contains data.

SDA ---- All Structure DAta (image, attributes, connection table and map table if it contains data).

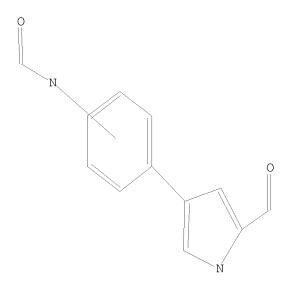
NOS ---- NO Structure data.

ENTER STRUCTURE FORMAT (SIA), SCT, SDA, SIM, SAT, NOS:sia

L11 STR



Structure attributes must be viewed using STN Express query preparation. L13 STR



Structure attributes must be viewed using STN Express query preparation.

L18 185 SEA FILE=REGISTRY SSS FUL L11

L23 16 SEA FILE=REGISTRY SUB=L18 SSS FUL L13 L24 8 SEA FILE=ZCAPLUS ABB=ON PLU=ON L23

L25 0 SEA FILE=ZCAPLUS ABB=ON PLU=ON L24 AND ?POLYAMID?

=> d 124 ibib hitstr 1-8

THE ESTIMATED COST FOR THIS REQUEST IS 31.12 U.S. DOLLARS DO YOU WANT TO CONTINUE WITH THIS REQUEST? (Y)/N: $\gamma$ 

L24 ANSWER 1 OF 8 ZCAPLUS COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 2009:20677 ZCAPLUS

DOCUMENT NUMBER: 150:97912

TITLE: Cycloalkylcarboxamides and related compounds as

modulators of ATP-binding cassette transporters and their preparation, pharmaceutical compositions and use

in the treatment of cystic fibrosis

INVENTOR(S): Hadida Ruah, Sara; Miller, Mark; Grootenhuis, Peter;

Bear, Brian; McCartney, Jason

PATENT ASSIGNEE(S): Vertex Pharmaceuticals Incorporated, USA

SOURCE: PCT Int. Appl., 254pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent LANGUAGE: English

FAMILY ACC. NUM. COUNT: 3

PATENT INFORMATION:

PA	PATENT NO.					KIND DATE			APPLICATION NO.						DATE			
WO	WO 2009006315				A1 20090108			0108	1	008-1	JS68	20080627						
	W:	ΑE,	AG,	AL,	AM,	AO,	ΑT,	ΑU,	AZ,	BA,	BB,	BG,	BH,	BR,	BW,	BY,	BZ,	
		CA,	CH,	CN,	CO,	CR,	CU,	CZ,	DE,	DK,	DM,	DO,	DZ,	EC,	EE,	EG,	ES,	
		FΙ,	GB,	GD,	GE,	GH,	GM,	GT,	HN,	HR,	HU,	ID,	IL,	IN,	IS,	JP,	KE,	
		KG,	ΚM,	KN,	KΡ,	KR,	KΖ,	LA,	LC,	LK,	LR,	LS,	LT,	LU,	LY,	MA,	MD,	
		ME,	MG,	MK,	MN,	MW,	MX,	MY,	MZ,	NA,	NG,	NΙ,	NO,	NΖ,	OM,	PG,	PH,	
		PL,	PT,	RO,	RS,	RU,	SC,	SD,	SE,	SG,	SK,	SL,	SM,	SV,	SY,	ТJ,	TM,	
		TN,	TR,	TT,	TZ,	UA,	UG,	US,	UΖ,	VC,	VN,	ZA,	ZM,	ZW				
	RW:	ΑT,	BE,	BG,	CH,	CY,	CZ,	DE,	DK,	EE,	ES,	FI,	FR,	GB,	GR,	HR,	HU,	
		ΙE,	IS,	ΙΤ,	LT,	LU,	LV,	MC,	MT,	NL,	NO,	PL,	PT,	RO,	SE,	SI,	SK,	
		TR,	BF,	ΒJ,	CF,	CG,	CI,	CM,	GΑ,	GN,	GQ,	GW,	${ m ML}$ ,	MR,	ΝE,	SN,	TD,	
		ΤG,	BW,	GH,	GM,	KΕ,	LS,	MW,	MZ,	NA,	SD,	SL,	SZ,	TZ,	UG,	ZM,	ZW,	
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US	US 20080009524						2008	0110	1	US 2007-824606				2007062				
PRIORIT	PRIORITY APPLN. INFO.:								1	US 2007-824606				A 2	0070	629		
									US 2005-		754558P			P 2	20051228			
									1	US 2	JS 2006-		302580P		P 2	0060	522	
							US 2006-647092						92		A2 2	.2 200612:		

OTHER SOURCE(S): MARPAT 150:97912

IT 945242-72-8P 945243-34-5P

RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(drug candidate; preparation of cycloalkylcarboxamides and related compds. as modulators of ATP-binding cassette transporters useful in the treatment of cystic fibrosis)

RN 945242-72-8 ZCAPLUS

CN 1H-Pyrrole-2-carboxylic acid, 4-[5-[[[1-(1,3-benzodioxol-5-yl)cyclopropyl]carbonyl]amino]-2-methylphenyl]- (CA INDEX NAME)

RN 945243-34-5 ZCAPLUS

CN 1H-Pyrrole-2-carboxylic acid, 4-[5-[[[1-(2,2-difluoro-1,3-benzodioxol-5-yl)cyclopropyl]carbonyl]amino]-2-methylphenyl]- (CA INDEX NAME)

3 THERE ARE 3 CITED REFERENCES AVAILABLE FOR THIS REFERENCE COUNT: RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L24 ANSWER 2 OF 8 ZCAPLUS COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 2008:43636 ZCAPLUS

DOCUMENT NUMBER: 148:121398

Cycloalkylcarboxamides and related compounds as TITLE:

> modulators of ATP-binding cassette transporters and their preparation, pharmaceutical compositions and use

in the treatment of diseases

INVENTOR(S): Hadida Ruah, Sara S.; Miller, Mark T.; Bear, Brian;

McCartney, Jason; Grootenhuis, Peter D. J.

PATENT ASSIGNEE(S):

SOURCE: U.S. Pat. Appl. Publ., 422 pp., Cont.-in-part of U.S.

Ser. No. 647,092.

CODEN: USXXCO

Patent DOCUMENT TYPE: English LANGUAGE:

FAMILY ACC. NUM. COUNT:

PATENT INFORMATION:

PA	PATENT NO.						KIND DATE			APPLICATION NO.					DATE			
US	2008	0009	 524		A1 20080110				US 2	:007-	 8246	20070629						
US	20080044355				A1 20080221					US 2	006-	6470	20061228					
WO	2009	0063	15		A1 200			0090108		WO 2	008-	609	20080627					
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		FI,	GB,	GD,	GE,	GH,	GM,	GT,	HN,	HR,	HU,	ID,	IL,	IN,	IS,	JP,	KE,	
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OTHER S	OURCE	(5) •			MZD.	PZT	148.	1213		00 2	.00/	0240	00			0070	029	
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945242-72-8P 945243-34-5P

RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES

(Uses)

(drug candidate; preparation of cycloalkylcarboxamides and related compds. as modulators of ATP-binding cassette transporters)

945242-72-8 ZCAPLUS RN

1H-Pyrrole-2-carboxylic acid, 4-[5-[[1-(1,3-benzodioxol-5-CN yl)cyclopropyl]carbonyl]amino]-2-methylphenyl]- (CA INDEX NAME)

945243-34-5 ZCAPLUS RN

1H-Pyrrole-2-carboxylic acid, 4-[5-[[[1-(2,2-difluoro-1,3-benzodioxol-5-CN yl)cyclopropyl]carbonyl]amino]-2-methylphenyl]- (CA INDEX NAME)

L24 ANSWER 3 OF 8 ZCAPLUS COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 2007:846121 ZCAPLUS

DOCUMENT NUMBER: 147:211534

TITLE: Cycloalkylcarboxamides and related compounds as

> modulators of ATP-binding cassette transporters and their preparation, pharmaceutical compositions and use

in the treatment of diseases

Ruah, Sara S. Hadida; Miller, Mark T.; Bear, Brian; INVENTOR(S):

> McCartney, Jason; Grootenhuis, Peter D. J. Vertex Pharmaceuticals Incorporated, USA

PATENT ASSIGNEE(S): SOURCE:

PCT Int. Appl., 249 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent LANGUAGE: English

FAMILY ACC. NUM. COUNT: 3

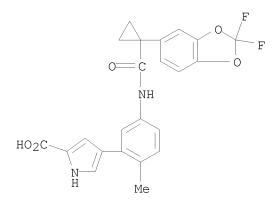
PATENT INFORMATION:

APPLICATION NO. PATENT NO. KIND DATE DATE \_\_\_\_\_

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WO 2007087066
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                                                                    20061228
     WO 2007087066
                          А3
                                20071025
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     AU 2006336504
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     JP 2009522277
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                                                                    20080825
PRIORITY APPLN. INFO.:
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                                                                    20051228
                                             US 2006-802580P
                                                                 Ρ
                                                                    20060522
                                             WO 2006-US49412
                                                                 W
                                                                    20061228
OTHER SOURCE(S):
                         MARPAT 147:211534
     945242-72-8P 945243-34-5P
     RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU
     (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES
     (Uses)
        (drug candidate; preparation of cycloalkylcarboxamides and related compds.
        as modulators of ATP-binding cassette transporters)
     945242-72-8 ZCAPLUS
RN
     1H-Pyrrole-2-carboxylic acid, 4-[5-[[1-(1,3-benzodioxol-5-
CN
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RN 945243-34-5 ZCAPLUS
CN 1H-Pyrrole-2-carboxylic acid, 4-[5-[[[1-(2,2-difluoro-1,3-benzodioxol-5-yl)cyclopropyl]carbonyl]amino]-2-methylphenyl]- (CA INDEX NAME)

yl)cyclopropyl]carbonyl]amino]-2-methylphenyl]- (CA INDEX NAME)



L24 ANSWER 4 OF 8 ZCAPLUS COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 2007:684665 ZCAPLUS

DOCUMENT NUMBER: 147:300934

TITLE: Indolinone based phosphoinositide-dependent kinase-1

(PDK1) inhibitors. Part 2: Optimization of BX-517 Islam, Imadul; Brown, Greg; Bryant, Judi; Hrvatin, Paul; Kochanny, Monica J.; Phillips, Gary B.; Yuan, Shendong; Adler, Marc; Whitlow, Marc; Lentz, Dao;

Shendong; Adler, Marc; Whitlow, Marc; Lentz, Dao; Polokoff, Mark A.; Wu, James; Shen, Jun; Walters, Janette; Ho, Elena; Subramanyam, Babu; Zhu, Daguang;

Feldman, Richard I.; Arnaiz, Damian O.

CORPORATE SOURCE: Berlex Biosciences, Richmond, CA, 94804, USA

SOURCE: Bioorganic & Medicinal Chemistry Letters (2007),

17(14), 3819-3825

CODEN: BMCLE8; ISSN: 0960-894X

PUBLISHER: Elsevier Ltd.

DOCUMENT TYPE: Journal LANGUAGE: English

OTHER SOURCE(S): CASREACT 147:300934

IT 946847-38-7P

AUTHOR(S):

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation, phosphoinositide-dependent kinase-1 inhibitory, anticancer activity, and SAR of (pyrrolylmethyliden)indolinones)

RN 946847-38-7 ZCAPLUS

CN Acetamide, N-[3-[5-formyl-1-[(4-methylphenyl)sulfonyl]-1H-pyrrol-3-yl]phenyl]- (CA INDEX NAME)

REFERENCE COUNT: 13 THERE ARE 13 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L24 ANSWER 5 OF 8 ZCAPLUS COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 2007:666267 ZCAPLUS

DOCUMENT NUMBER: 147:72808

TITLE: Preparation of pyrrolo[1,2-a]quinoxaline derivatives

as adenosine A3 receptor modulators

INVENTOR(S): Schann, Stephan; Mayer, Stanislas; Gardan, Sophie

PATENT ASSIGNEE(S): Faust Pharmaceuticals, Fr.

SOURCE: Eur. Pat. Appl., 25pp.

CODEN: EPXXDW

DOCUMENT TYPE: Patent LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND DATE	APPLICATION NO.	DATE
	A1 20070620	EP 2005-292739	20051219
R: AT, BE, BG,	CH, CY, CZ, DE,	DK, EE, ES, FI, FR, GB,	GR, HU, IE,
IS, IT, LI,	LT, LU, LV, MC,	NL, PL, PT, RO, SE, SI,	SK, TR, AL,
BA, HR, MK,	, YU		
AU 2006328934	A1 20070628	AU 2006-328934	20061219
CA 2634165	A1 20070628	CA 2006-2634165	20061219
WO 2007071379	A1 20070628	WO 2006-EP12258	20061219
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KP, KR, KZ,	, LA, LC, LK, LR,	LS, LT, LU, LV, LY, MA,	MD, MG, MK,
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RS, RU, SC,	, SD, SE, SG, SK,	SL, SM, SV, SY, TJ, TM,	TN, TR, TT,
TZ, UA, UG,	, US, UZ, VC, VN,	ZA, ZM, ZW	
RW: AT, BE, BG,	CH, CY, CZ, DE,	DK, EE, ES, FI, FR, GB,	GR, HU, IE,
IS, IT, LT,	LU, LV, MC, NL,	PL, PT, RO, SE, SI, SK,	TR, BF, BJ,
CF, CG, CI,	, CM, GA, GN, GQ,	GW, ML, MR, NE, SN, TD,	TG, BW, GH,
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EP 1973916	A1 20081001	EP 2006-841044	20061219
R: AT, BE, BG,	CH, CY, CZ, DE,	DK, EE, ES, FI, FR, GB,	GR, HU, IE,
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JP 2009519988	T 20090521	JP 2008-546234	20061219

US 20090093476 A1 20090409 US 2008-158035 20081031 PRIORITY APPLN. INFO.: EP 2005-292739 A 20051219 WO 2006-EP12258 W 20061219

OTHER SOURCE(S): MARPAT 147:72808

IT 941714-55-2P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation of pyrrolo[1,2-a]quinoxaline derivs. as adenosine A3 receptor modulators)

RN 941714-55-2 ZCAPLUS

CN 1H-Pyrrole-2-carboxylic acid, 4-[4-[[(1,1-

dimethylethoxy)carbonyl]amino]phenyl]-1-(2-nitrophenyl)-, methyl ester
(CA INDEX NAME)

REFERENCE COUNT: 6 THERE ARE 6 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L24 ANSWER 6 OF 8 ZCAPLUS COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 2005:1004692 ZCAPLUS

DOCUMENT NUMBER: 143:286420

TITLE: Preparation of aminobiaryl carboxylic acids for the

 $\hbox{\it manufacture of medicaments for treating proliferative}$ 

disease

INVENTOR(S): Howard, Philip Wilson; Wells, Geoffrey

PATENT ASSIGNEE(S): Spirogen Limited, UK SOURCE: PCT Int. Appl., 90 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2005085177	A2	20050915	WO 2005-GB752	20050301
W: AE, AG,	L, AM, AT,	AU, AZ, BA	, BB, BG, BR, BW,	BY, BZ, CA, CH,
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GE, GH,	M, HR, HU,	ID, IL, IN	, IS, JP, KE, KG,	KP, KR, KZ, LC,
LK, LR,	S, LT, LU,	LV, MA, MD	, MG, MK, MN, MW,	MX, MZ, NA, NI,
NO, NZ,	M, PG, PH,	PL, PT, RO	, RU, SC, SD, SE,	SG, SK, SL, SM,
SY, TJ,	M, TN, TR,	TT, TZ, UA	, UG, US, UZ, VC,	VN, YU, ZA, ZM, ZW
RW: BW, GH,	M, KE, LS,	MW, MZ, NA	, SD, SL, SZ, TZ,	UG, ZM, ZW, AM,
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EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG 20061206 EP 2005-717831 EP 1727808 20050301 Α2 20081112 EP 1727808 В1 R: AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LI, LT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR AT 414065 Τ 20081115 AT 2005-717831 20050301 US 20070249591 Α1 20071025 US 2007-591140 20070108 PRIORITY APPLN. INFO.: GB 2004-4574 A 20040301 WO 2005-GB752 W 20050301 OTHER SOURCE(S): CASREACT 143:286420; MARPAT 143:286420 864076-03-9P 864076-44-8P RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses) (preparation of aminobiaryl carboxylic acids for manufacture of medicaments for treating proliferative disease) RN 864076-03-9 ZCAPLUS CN 1H-Pyrrole-2-carboxylic acid, 4-[4-[(1,1dimethylethoxy)carbonyl]amino]phenyl]-1-methyl- (CA INDEX NAME)

RN 864076-44-8 ZCAPLUS

CN 1H-Pyrrole-2-carboxylic acid, 4-[4-[[4-[[4-[[4-(dimethylamino)-1-oxobutyl]amino]-1-methyl-1H-pyrrol-2-yl]carbonyl]amino]-1-methyl-1H-pyrrol-2-yl]carbonyl]amino]phenyl]-1-methyl-, methyl ester (CA INDEX NAME)

IT 864076-02-8P 864076-32-4P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation of aminobiaryl carboxylic acids for manufacture of medicaments

for

treating proliferative disease)

RN 864076-02-8 ZCAPLUS

CN 1H-Pyrrole-2-carboxylic acid, 4-[4-[[(1,1-dimethylethoxy)carbonyl]amino]phenyl]-1-methyl-, methyl ester (CA INDEX NAME)

RN 864076-32-4 ZCAPLUS

CN 1H-Pyrrole-2-carboxylic acid, 4-[4-[[4-[[[4-[[[4-[[(1,1-dimethylethoxy)carbonyl]amino]-1-methyl-1H-pyrrol-2-yl]carbonyl]amino]-1-methyl-1H-pyrrol-2-yl]carbonyl]amino]phenyl]-1-methyl-, methyl ester (CA INDEX NAME)

REFERENCE COUNT: 2 THERE ARE 2 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L24 ANSWER 7 OF 8 ZCAPLUS COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 2004:570508 ZCAPLUS

DOCUMENT NUMBER: 141:106366

TITLE: Preparation of substituted pyrroles as kinase

inhibitors

INVENTOR(S): Sun, Connie Li; Tang, Peng Cho; Ockey, Denise

PATENT ASSIGNEE(S): Sugen, Inc., USA

SOURCE: U.S. Pat. Appl. Publ., 44 pp.

CODEN: USXXCO

DOCUMENT TYPE: Patent LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 20040138269 PRIORITY APPLN. INFO.:	A1	20040715	US 2003-679693 US 2002-417555P	20031007
OTHER SOURCE(S):	MARPAT	141:106366		
IT 720708-39-4P, 3,5-D	imethyl	4-[3-(4-		
trifluoromethylbenz	oylamin	o)phenyl]-1H	I-pyrrole-2-carboxylic a	acid Ethyl
			pylphenyl)ureido]pheny.	
(toluene-4-sulfonyl	)-1H-py	rrole-2-carb	ooxylic Acid Benzyl Este	er
720708-52-1P, 1-(To	luene-4	-sulfonyl)-4	-[3-[N'-(2-	
	_		.H-pyrrole-2-carboxylic	Acid Benzyl
Ester 720708-54-3P,			<b>-</b>	
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•			4-yl)ureido]phenyl]-1	
<b>-</b>			ooxylic acid Benzyl Este	er
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pyrrole-2-carboxyli				
	_		'N (Synthetic preparation	
<u> </u>	BIOL (E	Siological st	udy); PREP (Preparation	n); USES
(Uses)				
(substituted pyr		ıs kinase inh	ibitors)	
RN 720708-39-4 ZCAPLU	-			
CN 1H-Pyrrole-2-carbox	ylic ac	id, 3,5-dime	thyl-4-[3-[[4-	

(trifluoromethyl)benzoyl]amino]phenyl]-, ethyl ester (CA INDEX NAME)

RN 720708-48-5 ZCAPLUS

CN 1H-Pyrrole-2-carboxylic acid, 4-[4-[[[[4-(1-methylethyl)phenyl]amino]carbonyl]amino]phenyl]-1-[(4-methylphenyl)sulfonyl]-, phenylmethyl ester (CA INDEX NAME)

PAGE 1-A

PAGE 2-A

RN

CN 1H-Pyrrole-2-carboxylic acid, 1-[(4-methylphenyl)sulfonyl]-4-[3-[[[[2-(trifluoromethyl)phenyl]amino]carbonyl]amino]phenyl]-, phenylmethyl ester (CA INDEX NAME)

RN 720708-54-3 ZCAPLUS

CN 1H-Pyrrole-2-carboxylic acid, 1-[(4-methylphenyl)sulfonyl]-4-[3-[[[[4-(trifluoromethyl)phenyl]amino]carbonyl]amino]phenyl]-, phenylmethyl ester (CA INDEX NAME)

RN 720708-55-4 ZCAPLUS

CN 1H-Pyrrole-2-carboxylic acid, 4-[3-[[([1,1'-biphenyl]-4-ylamino)carbonyl]amino]phenyl]-1-[(4-methylphenyl)sulfonyl]-, phenylmethyl ester (CA INDEX NAME)

RN 720708-57-6 ZCAPLUS

CN 1H-Pyrrole-2-carboxamide, 4-[4-[[[[4-(1-methylethyl)phenyl]amino]carbonyl]amino]phenyl]-N-[2-(4-morpholinyl)ethyl](CA INDEX NAME)

L24 ANSWER 8 OF 8 ZCAPLUS COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 2000:498632 ZCAPLUS

DOCUMENT NUMBER: 133:281935

TITLE: Synthesis of a rhazinilam analogue acting as an

inhibitor of tubulin assembly

AUTHOR(S): Dupont, C.; Guenard, D.; Thal, C.; Thoret, S.;

Gueritte, F.

CORPORATE SOURCE: Institut de Chimie des Substances Naturelles, Centre

National de la Recherche Scientifique, Gif-sur-Yvette,

91198, Fr.

SOURCE: Tetrahedron Letters (2000), 41(31), 5853-5856

CODEN: TELEAY; ISSN: 0040-4039

PUBLISHER: Elsevier Science Ltd.

DOCUMENT TYPE: Journal LANGUAGE: English

OTHER SOURCE(S): CASREACT 133:281935

IT 299918-29-9P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation of rhazinilam anal as inhibitor of tubulin assembly)

RN 299918-29-9 ZCAPLUS

CN 1H-Pyrrole-2-carboxylic acid, 5-(1-cyano-1-ethylpropyl)-4-[2-[[(1,1-dimethylethoxy)carbonyl]amino]phenyl]-1-methyl-, methyl ester (CA INDEX NAME)

IT 299918-28-8P

RL: SPN (Synthetic preparation); PREP (Preparation) (preparation of rhazinilam anal as inhibitor of tubulin assembly)

RN 299918-28-8 ZCAPLUS

CN 1H-Pyrrole-2-carboxylic acid, 5-(cyanomethyl)-4-[2-[[(1,1-dimethylethoxy)carbonyl]amino]phenyl]-1-methyl-, methyl ester (CA INDEX NAME)

REFERENCE COUNT: 18 THERE ARE 18 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

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SUBSET AND SAMPLE ARE IGNORED FOR THIS SEARCH

1 US2007-591140/AP

0 US2007-591140/PRN L26 1 US2007-591140/APPS

(US2007-591140/AP,PRN)

=> file registry
COST IN U.S. DOLLARS

SINCE FILE

TOTAL

FULL ESTIMATED COST ENTRY SESSION 43.25 335.05

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STRUCTURE FILE UPDATES: 16 JUN 2009 HIGHEST RN 1158716-03-0 DICTIONARY FILE UPDATES: 16 JUN 2009 HIGHEST RN 1158716-03-0

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Please note that search-term pricing does apply when conducting  ${\tt SmartSELECT}$  searches.

REGISTRY includes numerically searchable data for experimental and predicted properties as well as tags indicating availability of experimental property data in the original document. For information on property searching in REGISTRY, refer to:

http://www.cas.org/support/stngen/stndoc/properties.html

=> s l1 sam sub=L18
SUBSET AND SAMPLE ARE IGNORED FOR THIS SEARCH
'APPS' IS NOT A VALID FIELD CODE
L27 0 US2007-591140/APPS

=> s 13 sam sub=L18
SAMPLE SUBSET SEARCH INITIATED 17:20:54 FILE 'REGISTRY'
SAMPLE SUBSET SCREEN SEARCH COMPLETED - 7 TO ITERATE

100.0% PROCESSED 7 ITERATIONS 7 ANSWERS SEARCH TIME: 00.00.01

PROJECTIONS (WITHIN SPECIFIED SUBSET): ONLINE \*\*COMPLETE\*\*
PROJECTED ITERATIONS (WITHIN SPECIFIED SUBSET): 7 TO 298
PROJECTED ANSWERS (WITHIN SPECIFIED SUBSET): 7 TO 298

L28 7 SEA SUB=L18 SSS SAM L3

=> d sca

\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

L28 7 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN IN 1H-Pyrrole-2-carboxylic acid, 4-[4-[[(2,6-dichlorophenyl)methyl]amino]phenyl]-1-octyl-MF C26 H30 C12 N2 O2

\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

L28 7 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN

 $1 \\ H-Pyrrole-2-carboxylic acid, 1-[(2-chlorophenyl)methyl]-4-[4-[[(3,5-chlorophenyl)methyl]]-4-[4-[(3,5-chlorophenyl)methyl]$ ΙN difluorophenyl)methyl]amino]phenyl]-, methyl ester

MF C26 H21 C1 F2 N2 O2

PAGE 1-A

PAGE 2-A

\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

REGISTRY COPYRIGHT 2009 ACS on STN L28 7 ANSWERS

1H-Pyrrole-2-carboxylic acid, 5-nitro-4-(4-nitrophenyl)-, ethyl ester ΙN

MFC13 H11 N3 O6

\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

L28 7 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN IN 1H-Pyrrole-2-carboxylic acid, 4-(4-aminophenyl)-1-hexyl-, methyl ester MF C18 H24 N2 O2

\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

L28 7 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN
IN 1H-Pyrrole-2-carboxylic acid, 4-(4-aminophenyl)-1-methyl-, methyl ester
MF C13 H14 N2 O2

\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

L28 7 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN

IN 1H-Pyrrole-2-carboxylic acid, 4-(4-aminophenyl)-1-[(2-chlorophenyl)methyl]-1

, methyl ester

MF C19 H17 C1 N2 O2

\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

ALL ANSWERS HAVE BEEN SCANNED

=> s 13 full (sss) sub=L18
COMBINATION OF STRUCTURE AND TEXT TERMS NOT VALID
The query entered contains both search terms created by
structure-building or screen commands and text search terms. L#s
created via the STRUCTURE or SCREEN commands must be searched in the
structures files separately from text terms or profiles. The L#
answer sets from structure searches can be used in crossover searches
and can be combined with text terms.

=> s 13 full sub=L18 THE ESTIMATED SEARCH COST FOR FILE 'REGISTRY' IS 44.00 U.S. DOLLARS DO YOU WANT TO CONTINUE WITH THIS REQUEST? (Y)/N or END:y FULL SUBSET SEARCH INITIATED 17:22:57 FILE 'REGISTRY' FULL SUBSET SCREEN SEARCH COMPLETED -102 TO ITERATE

97 ANSWERS 100.0% PROCESSED 102 ITERATIONS

SEARCH TIME: 00.00.01

L29 97 SEA SUB=L18 SSS FUL L3

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SINCE FILE TOTAL ENTRY SESSION FULL ESTIMATED COST 47.84 382.89

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This file contains CAS Registry Numbers for easy and accurate substance identification.

=> s 129

L30 17 L29

=> s 130 and ?polyamid? 201293 ?POLYAMID? L31 0 L30 AND ?POLYAMID?

=> s 130 not 124

L32 14 L30 NOT L24

=> d 132 ibib hitstr 4-14 THE ESTIMATED COST FOR THIS REQUEST IS 42.79 U.S. DOLLARS DO YOU WANT TO CONTINUE WITH THIS REQUEST? (Y)/N:n REQUEST CANCELED

=> d 132 ibib hitstr 10-14
THE ESTIMATED COST FOR THIS REQUEST IS 19.45 U.S. DOLLARS
DO YOU WANT TO CONTINUE WITH THIS REQUEST? (Y)/N:y

L32 ANSWER 10 OF 14 ZCAPLUS COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 1970:506610 ZCAPLUS

DOCUMENT NUMBER: 73:106610

ORIGINAL REFERENCE NO.: 73:17353a,17356a

TITLE: Total synthesis of pyrrolnitrin. XI.

Structure-activity studies of pyrrolnitrin analogs
AUTHOR(S):
Umio, Suminori; Kariyone, Kazuo; Tanaka, Kunihiko;
Kishimoto, Teiji; Nakamura, Hitoshi; Nishida, Minoru

CORPORATE SOURCE: Res. Lab., Fujisawa Pharm. Co., Ltd., Osaka, Japan SOURCE: Chemical & Pharmaceutical Bulletin (1970), 18(7),

1414-25

CODEN: CPBTAL; ISSN: 0009-2363

DOCUMENT TYPE: Journal LANGUAGE: English IT 16385-04-9P 16385-10-7P

RL: SPN (Synthetic preparation); PREP (Preparation)

(preparation of) 16385-04-9 ZCAPLUS

CN 1H-Pyrrole-2,5-dicarboxylic acid, 3-chloro-4-(2-chloro-4-nitrophenyl)-, 5-ethyl ester (CA INDEX NAME)

RN

RN 16385-10-7 ZCAPLUS

CN 1H-Pyrrole-2,5-dicarboxylic acid, 3-chloro-4-(4-nitrophenyl)-, 5-ethyl ester (CA INDEX NAME)

L32 ANSWER 11 OF 14 ZCAPLUS COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 1968:443795 ZCAPLUS

DOCUMENT NUMBER: 69:43795

ORIGINAL REFERENCE NO.: 69:8202h,8203a

3-Halo-4-phenylpyrrole-2,5-dicarboxylic acids TITLE:

INVENTOR(S): Umio, Suminori; Kariyone, Kazuo; Tanaka, Kunihiko;

Kishimoto, Teiji

Fujisawa Pharmaceutical Co., Ltd. PATENT ASSIGNEE(S):

SOURCE: Jpn. Tokkyo Koho, 4 pp.

CODEN: JAXXAD

DOCUMENT TYPE: Patent LANGUAGE: Japanese

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO. KIND DATE APPLICATION NO. DATE \_\_\_\_ JP 42017820 В4 19670918 JP 19641224

18488-76-1P 19283-37-5P ΤT

RL: SPN (Synthetic preparation); PREP (Preparation)

(preparation of)

18488-76-1 ZCAPLUS RN

1H-Pyrrole-2,5-dicarboxylic acid, 3-chloro-4-(2-chloro-4-nitrophenyl)-CN (CA INDEX NAME)

19283-37-5 ZCAPLUS RN

1H-Pyrrole-2,5-dicarboxylic acid, 3-chloro-4-(4-nitrophenyl)- (CA INDEX CN NAME)

L32 ANSWER 12 OF 14 ZCAPLUS COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 1968:87148 ZCAPLUS

DOCUMENT NUMBER: 68:87148

ORIGINAL REFERENCE NO.: 68:16795a,16798a TITLE: Phenylpyrroles

INVENTOR(S): Umio, Suminori; Kariyone, Kazuo; Tanaka, Kunihiko;

Kishimoto, Teiji

PATENT ASSIGNEE(S): Fujisawa Pharmaceutical Co., Ltd.

SOURCE: Fr., 14 pp. CODEN: FRXXAK

DOCUMENT TYPE: Patent LANGUAGE: French

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
FR 1472991		19670317	FR 1965-33177	19650929
DE 1545861			DE	
GB 1127929			GB	
JP 42017820		19670000	JP	
JP 42024414		19670000	JP	
US 3428648		19690218	US	19670320
US 3487089		19691230	US	19680130
PRIORITY APPLN. INFO.:			JP	19641224
			JP	19650408

IT 16385-04-9P 18488-76-1P

RN 16385-04-9 ZCAPLUS

CN 1H-Pyrrole-2,5-dicarboxylic acid, 3-chloro-4-(2-chloro-4-nitrophenyl)-, 5-ethyl ester (CA INDEX NAME)

RN 18488-76-1 ZCAPLUS

CN 1H-Pyrrole-2,5-dicarboxylic acid, 3-chloro-4-(2-chloro-4-nitrophenyl)- (CA INDEX NAME)

L32 ANSWER 13 OF 14 ZCAPLUS COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 1967:516814 ZCAPLUS

DOCUMENT NUMBER: 67:116814

ORIGINAL REFERENCE NO.: 67:22003a,22006a

TITLE: 3-Chloro-4-phenylpyrrole-2-carboxylic acids

INVENTOR(S): Umio, Suminori; Kariyone, Kazuo; Tanaka, Kunihiko;

Kishimoto, Teiji

PATENT ASSIGNEE(S): Fujisawa Pharmaceutical Co., Ltd.

SOURCE: Jpn. Tokkyo Koho, 5 pp.

CODEN: JAXXAD

DOCUMENT TYPE: Patent LANGUAGE: Japanese

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 42008863	B4	19670425	JP	19641207
US 3487089		19691230	US	19680130

IT 16385-04-9P 16385-10-7P

RL: SPN (Synthetic preparation); PREP (Preparation)

(preparation of)

RN 16385-04-9 ZCAPLUS

CN 1H-Pyrrole-2,5-dicarboxylic acid, 3-chloro-4-(2-chloro-4-nitrophenyl)-, 5-ethyl ester (CA INDEX NAME)

RN 16385-10-7 ZCAPLUS

CN 1H-Pyrrole-2,5-dicarboxylic acid, 3-chloro-4-(4-nitrophenyl)-, 5-ethyl ester (CA INDEX NAME)

L32 ANSWER 14 OF 14 ZCAPLUS COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 1967:482091 ZCAPLUS

DOCUMENT NUMBER: 67:82091

ORIGINAL REFERENCE NO.: 67:15471a,15474a

TITLE: 3-Substituted phenylpyrrole-2,5-dicarboxylic acid

derivatives

INVENTOR(S): Umio, Suminori; Kariyone, Kazuo; Tanaka, Kunihiko

PATENT ASSIGNEE(S): Fujisawa Pharmaceutical Co., Ltd.

SOURCE: Jpn. Tokkyo Koho, 3 pp.

CODEN: JAXXAD

DOCUMENT TYPE: Patent LANGUAGE: Japanese

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 42004588	В4	19670224	JP	19641023

IT 16121-71-4P

RL: SPN (Synthetic preparation); PREP (Preparation)

(preparation of)

RN 16121-71-4 ZCAPLUS

CN 1H-Pyrrole-2,5-dicarboxylic acid, 3-(4-nitrophenyl)-, 2,5-dimethyl ester (CA INDEX NAME)

=> s 132 not NO2 152533 NO2

L33 10 L32 NOT NO2

=> d 132 ibib hitstr 5-9

THE ESTIMATED COST FOR THIS REQUEST IS 19.45 U.S. DOLLARS DO YOU WANT TO CONTINUE WITH THIS REQUEST? (Y)/N:y

L32 ANSWER 5 OF 14 ZCAPLUS COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 2003:551493 ZCAPLUS

DOCUMENT NUMBER: 139:117337

TITLE: Preparation of pyrrole derivatives as androgen

receptor antagonists

INVENTOR(S): Furuya, Shuichi; Matsunaga, Nobuyuki; Kusaka, Masami;

Hara, Takahito; Miyazaki, Junichi

PATENT ASSIGNEE(S): Takeda Chemical Industries, Ltd., Japan

SOURCE: PCT Int. Appl., 306 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent LANGUAGE: Japanese

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND DATE	APPLICATION NO.	DATE
WO 2003057669	A1 20030717	WO 2002-JP13652	20021226
W: AE, AG, AL,	AM, AT, AU, AZ,	BA, BB, BG, BR, BY, BZ,	CA, CH, CN,
CO, CR, CU,	CZ, DE, DK, DM,	DZ, EC, EE, ES, FI, GB,	GD, GE, GH,
GM, HR, HU,	ID, IL, IN, IS,	JP, KE, KG, KR, KZ, LC,	LK, LR, LS,
LT, LU, LV,	MA, MD, MG, MK,	MN, MW, MX, MZ, NO, NZ,	OM, PH, PL,

PT, RO, RU, SC, SD, SE, SG, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG CA 2471754 Α1 20030717 CA 2002-2471754 20021226 AU 2002367424 AU 2002-367424 Α1 20030724 20021226 JP 2003252854 20030910 JP 2002-378462 20021226 EP 1466902 20041013 EP 2002-790889 20021226 Α1 AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, SK US 20050101657 Α1 20050512 US 2004-499300 20040618 PRIORITY APPLN. INFO.: JP 2001-399143 A 20011228 WO 2002-JP13652 W 20021226

OTHER SOURCE(S): MARPAT 139:117337

IT 562072-38-2P 562072-39-3P

RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(preparation of pyrrole derivs. as androgen receptor antagonists for preventive and therapeutic drugs for hormone-dependent cancers, in particular prostate cancer)

RN 562072-38-2 ZCAPLUS

CN 1H-Pyrrole-2-carboxylic acid, 3,5-dimethyl-4-(4-nitrophenyl)-, ethyl ester (CA INDEX NAME)

RN 562072-39-3 ZCAPLUS

CN 1H-Pyrrole-2-carboxylic acid, 3,5-dimethyl-4-(4-nitrophenyl)-1-(phenylmethyl)-, ethyl ester (CA INDEX NAME)

REFERENCE COUNT: 4 THERE ARE 4 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L32 ANSWER 6 OF 14 ZCAPLUS COPYRIGHT 2009 ACS on STN

2000:45653 ZCAPLUS ACCESSION NUMBER:

DOCUMENT NUMBER: 132:160970

TITLE: Synthesis and cytotoxicity of 2,4-disubstituted and

2,3,4-trisubstituted brominated pyrroles in murine and

human cultured tumor cells

Gupton, John T.; Burham, Bruce S.; Krumpe, Keith; Du, AUTHOR(S):

Karen; Sikorski, James A.; Warren, Amy E.; Barnes,

Cheryl R.; Hall, Iris H.

CORPORATE SOURCE: Dep. Chemistry, Univ. North Carolina, Asheville, NC,

28804, USA

SOURCE: Archiv der Pharmazie (Weinheim, Germany) (2000),

333(1), 3-9

CODEN: ARPMAS; ISSN: 0365-6233

PUBLISHER: Wiley-VCH Verlag GmbH

DOCUMENT TYPE: Journal LANGUAGE: English

258504-87-9P

RL: BAC (Biological activity or effector, except adverse); BSU (Biological

study, unclassified); SPN (Synthetic preparation); BIOL (Biological

study); PREP (Preparation)

(preparation and antitumor activity of brominated pyrroles)

RN 258504-87-9 ZCAPLUS

1H-Pyrrole-2-carboxylic acid, 3,5-dibromo-1-methyl-4-(4-nitrophenyl)-, CN

ethyl ester (CA INDEX NAME)

ΙT 127572-52-5

> RL: RCT (Reactant); RACT (Reactant or reagent) (preparation and antitumor activity of brominated pyrroles)

127572-52-5 ZCAPLUS RN

1H-Pyrrole-2-carboxylic acid, 1-methyl-4-(4-nitrophenyl)-, ethyl ester CN

(CA INDEX NAME)

REFERENCE COUNT: 36 THERE ARE 36 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L32 ANSWER 7 OF 14 ZCAPLUS COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 1994:435237 ZCAPLUS

DOCUMENT NUMBER: 121:35237

ORIGINAL REFERENCE NO.: 121:6499a,6502a
TITLE: Synthesis of methyl

3-aryl-4-trifluoromethyl-1H-pyrrole-2-carboxylates AUTHOR(S): La Porta, Piero; Capuzzi, Luigi; Bettarini, Franco

CORPORATE SOURCE: Isagro s.r.l., Novara, I-28100, Italy

SOURCE: Synthesis (1994), (3), 287-90

CODEN: SYNTBF; ISSN: 0039-7881

DOCUMENT TYPE: Journal LANGUAGE: English

OTHER SOURCE(S): CASREACT 121:35237

IT 155788-08-2P

RN

RL: SPN (Synthetic preparation); PREP (Preparation)

(preparation of) 155788-08-2 ZCAPLUS

CN 1H-Pyrrole-2-carboxylic acid, 1-(1,1-dimethylethyl)-4-(4-nitrophenyl)-3-(trifluoromethyl)-, methyl ester (CA INDEX NAME)

L32 ANSWER 8 OF 14 ZCAPLUS COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 1990:458830 ZCAPLUS

DOCUMENT NUMBER: 113:58830

ORIGINAL REFERENCE NO.: 113:9943a,9946a

TITLE: Application of 2-substituted vinamidinium salts to the

synthesis of 2,4-disubstituted pyrroles

AUTHOR(S): Gupton, John T.; Krolikowski, Dale A.; Yu, Richard H.;

Riesinger, Steve W.; Sikorski, James A.

CORPORATE SOURCE: Dep. Chem., Univ. Cent. Florida, Orlando, FL, 32816,

USA

SOURCE: Journal of Organic Chemistry (1990), 55(15), 4735-40

CODEN: JOCEAH; ISSN: 0022-3263

DOCUMENT TYPE: Journal LANGUAGE: English

OTHER SOURCE(S): CASREACT 113:58830

IT 127572-52-5P 127572-62-7P

RL: SPN (Synthetic preparation); PREP (Preparation)

(preparation of)

RN 127572-52-5 ZCAPLUS

CN 1H-Pyrrole-2-carboxylic acid, 1-methyl-4-(4-nitrophenyl)-, ethyl ester

(CA INDEX NAME)

RN 127572-62-7 ZCAPLUS

CN 1H-Pyrrole-2-carboxylic acid, 4-(4-nitrophenyl)-, ethyl ester (CA INDEX NAME)

L32 ANSWER 9 OF 14 ZCAPLUS COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 1970:520445 ZCAPLUS

DOCUMENT NUMBER: 73:120445

ORIGINAL REFERENCE NO.: 73:19623a,19626a

TITLE: Synthesis of pyrrolnitrin analogs. II. Preparation

antibacterial properties of

4-p-nitrophenyl-1-phenylpyrrole derivatives
AUTHOR(S): Artico, Marino; Filacchioni, Guido; Nacci, Vito;

Chimenti, Franco; Giardina, M. C.

CORPORATE SOURCE: Ist. Chim. Fram. Tossicol., Univ. Roma, Rome, Italy SOURCE: Farmaco, Edizione Scientifica (1970), 25(9), 651-68

CODEN: FRPSAX; ISSN: 0430-0920

DOCUMENT TYPE: Journal LANGUAGE: Italian

OTHER SOURCE(S): CASREACT 73:120445

IT 28993-09-1 28993-13-7

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); BIOL (Biological study)

(bactericidal activity of)

RN 28993-09-1 ZCAPLUS

CN 1H-Pyrrole-3-carboxylic acid, 5-cyano-2-formyl-4-(4-nitrophenyl)-1-phenyl-, ethyl ester (CA INDEX NAME)

RN 28993-13-7 ZCAPLUS

CN 1H-Pyrrole-2-carbonitrile, 4-chloro-5-formyl-3-(4-nitrophenyl)-1-phenyl-(CA INDEX NAME)

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FULL ESTIMATED COST

SINCE FILE TOTAL ENTRY SESSION 45.33 428.22

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STRUCTURE FILE UPDATES: 16 JUN 2009 HIGHEST RN 1158716-03-0 DICTIONARY FILE UPDATES: 16 JUN 2009 HIGHEST RN 1158716-03-0

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http://www.cas.org/support/stngen/stndoc/properties.html

=> s 129 not CAPLUS/LC 66966008 CAPLUS/LC

L34 1 L29 NOT CAPLUS/LC

=> d sca

L34 1 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN

1H-Pyrrole-2-carboxylic acid, 5-nitro-4-(4-nitrophenyl)-, ethyl ester

C13 H11 N3 O6 MF

\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

ALL ANSWERS HAVE BEEN SCANNED

=> file zcaplus COST IN U.S. DOLLARS

FULL ESTIMATED COST

SINCE FILE TOTAL ENTRY SESSION 5.83 434.05

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ZCAplus now includes complete International Patent Classification (IPC) reclassification data for the third quarter of 2008.

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This file contains CAS Registry Numbers for easy and accurate substance identification.

=> d 132 ibib hitstr 1-4 THE ESTIMATED COST FOR THIS REQUEST IS 15.56 U.S. DOLLARS DO YOU WANT TO CONTINUE WITH THIS REQUEST? (Y)/N:y

L32 ANSWER 1 OF 14 ZCAPLUS COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 2009:399344 ZCAPLUS

DOCUMENT NUMBER: 150:472520

TITLE: One-Pot Double Suzuki-Miyaura Couplings: Rapid Access

to Nonsymmetrical Tri(hetero)aryl Derivatives

AUTHOR(S): Beaumard, Floriane; Dauban, Philippe; Dodd, Robert H.

CORPORATE SOURCE: UPR 2301 CNRS, Institut de Chimie des Substances

Naturelles, Gif-sur-Yvette, 91198, Fr. Organic Letters (2009), 11(8), 1801-1804

CODEN: ORLEF7; ISSN: 1523-7060

PUBLISHER: American Chemical Society

DOCUMENT TYPE: Journal LANGUAGE: English

IT 1146731-61-4P

SOURCE:

RL: SPN (Synthetic preparation); PREP (Preparation)

(preparation of nonsym. tri(hetero)arenes via one-pot double Suzuki-Miyaura coupling of sym. dibromo(hetero)arenes with two different (hetero)aryl

boronic acids)

RN 1146731-61-4 ZCAPLUS

CN 1H-Pyrrole-2,5-dicarboxylic acid, 3-(4-nitrophenyl)-4-(3,4,5-trimethoxyphenyl)-, 2,5-diethyl ester (CA INDEX NAME)

PAGE 2-A

REFERENCE COUNT: 51 THERE ARE 51 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L32 ANSWER 2 OF 14 ZCAPLUS COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 2008:1383654 ZCAPLUS

DOCUMENT NUMBER: 149:575981

TITLE: The Vilsmeier reaction of fully conjugated carbocycles

and heterocycles

AUTHOR(S): Jones, Gurnos; Stanforth, Stephen P.

CORPORATE SOURCE: University Keele, Keele, UK

SOURCE: Organic Reactions (Hoboken, NJ, United States) (1997),

49, No pp. given CODEN: ORHNBA

URL: http://www3.interscience.wiley.com/cgi-

bin/mrwhome/107610747/HOME

PUBLISHER: John Wiley & Sons, Inc.

DOCUMENT TYPE: Journal; General Review; (online computer file)

LANGUAGE: English

OTHER SOURCE(S): CASREACT 149:575981

IT 1071118-60-9

RL: RCT (Reactant); RACT (Reactant or reagent)

(The Vilsmeier Reaction of Fully Conjugated Carbocycles and

Heterocycles)

RN 1071118-60-9 ZCAPLUS

CN 1H-Pyrrole-2-carboxylic acid, 3-methyl-4-(4-nitrophenyl)-, ethyl ester (CA INDEX NAME)

IT 1071118-63-2P

RL: SPN (Synthetic preparation); PREP (Preparation) (The Vilsmeier Reaction of Fully Conjugated Carbocycles and Heterocycles)

RN 1071118-63-2 ZCAPLUS

CN 1H-Pyrrole-2-carboxylic acid, 5-formyl-3-methyl-4-(4-nitrophenyl)-, ethyl ester (CA INDEX NAME)

L32 ANSWER 3 OF 14 ZCAPLUS COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 2008:176072 ZCAPLUS

DOCUMENT NUMBER: 148:285041

TITLE: Preparation of pyrrole derivatives as inhibitors of

fatty acid synthase for treating bacterial infection INVENTOR(S):
Li, Song; Zhang, Xuehui; Yu, Hong; Wang, Lili; Liu, Hongying; Zheng, Zhibing; Xie, Yunde; Zhong, Wu; Xiao,

Junhai; Li, Xingzhou; Cui, Hao

PATENT ASSIGNEE(S): Institute of Pharmacology and Toxicology, Academy of

Military Medical Sciences, The Chinese People's

Liberation Army, Peop. Rep. China

SOURCE: Faming Zhuanli Shenqing Gongkai Shuomingshu, 67pp.

CODEN: CNXXEV

DOCUMENT TYPE: Patent LANGUAGE: Chinese

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
CN 101117328	А	20080206	CN 2006-10104017	20060801
PRIORITY APPLN. INFO.:			CN 2006-10104017	20060801

OTHER SOURCE(S): CASREACT 148:285041; MARPAT 148:285041

IT 1008763-55-0P 1008763-56-1P 1008763-57-2P 1008763-58-3P 1008763-59-4P 1008763-60-7P

CN 1H-Pyrrole-2-carboxylic acid, 1-[(6-chloro-1,3-benzodioxol-5-yl)methyl]-4-[4-[[(2,6-dichlorophenyl)methyl]amino]phenyl]- (CA INDEX NAME)

RN 1008763-56-1 ZCAPLUS

CN 1H-Pyrrole-2-carboxylic acid, 1-[(2-chlorophenyl)methyl]-4-[4-[[(2,6-dichlorophenyl)methyl]amino]phenyl]- (CA INDEX NAME)

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- RN 1008763-57-2 ZCAPLUS
- CN 1H-Pyrrole-2-carboxylic acid, 1-[(3-chlorophenyl)methyl]-4-[4-[[(2,6-dichlorophenyl)methyl]amino]phenyl]- (CA INDEX NAME)

PAGE 1-A

PAGE 2-A

- RN 1008763-58-3 ZCAPLUS
- CN 1H-Pyrrole-2-carboxylic acid, 1-[(4-chlorophenyl)methyl]-4-[4-[(2,6-dichlorophenyl)methyl]amino]phenyl]- (CA INDEX NAME)

PAGE 2-A

RN 1008763-59-4 ZCAPLUS

CN 1H-Pyrrole-2-carboxylic acid, 4-[4-[[(2,6-dichlorophenyl)methyl]amino]phenyl]-1-pentyl- (CA INDEX NAME)

RN 1008763-60-7 ZCAPLUS
CN 1H-Pyrrole-2-carboxylic acid, 4-[4-[[(2,6-dichlorophenyl)methyl]amino]phenyl]-1-hexyl- (CA INDEX NAME)

RN 1008763-61-8 ZCAPLUS
CN 1H-Pyrrole-2-carboxylic acid, 4-[4-[[(2,6-dichlorophenyl)methyl]amino]phenyl]-1-heptyl- (CA INDEX NAME)

RN 1008763-62-9 ZCAPLUS
CN 1H-Pyrrole-2-carboxylic acid, 4-[4-[[(2,6-dichlorophenyl)methyl]amino]phenyl]-1-octyl- (CA INDEX NAME)

RN 1008763-63-0 ZCAPLUS

CN 1H-Pyrrole-2-carboxylic acid, 1-[(6-chloro-1,3-benzodioxol-5-yl)methyl]-4-[(3,5-difluorophenyl)methyl]amino]phenyl]- (CA INDEX NAME)

RN 1008763-64-1 ZCAPLUS

CN 1H-Pyrrole-2-carboxylic acid, 1-[(2-chlorophenyl)methyl]-4-[4-[[(3,5-difluorophenyl)methyl]amino]phenyl]- (CA INDEX NAME)

RN 1008763-65-2 ZCAPLUS

CN 1H-Pyrrole-2-carboxylic acid, 1-[(3-chlorophenyl)methyl]-4-[4-[[(3,5-difluorophenyl)methyl]amino]phenyl]- (CA INDEX NAME)

PAGE 2-A

RN 1008763-66-3 ZCAPLUS

CN 1H-Pyrrole-2-carboxylic acid, 1-[(4-chlorophenyl)methyl]-4-[4-[[(3,5-difluorophenyl)methyl]amino]phenyl]- (CA INDEX NAME)

PAGE 2-A

RN 1008763-67-4 ZCAPLUS

CN 1H-Pyrrole-2-carboxylic acid, 4-[4-[[(3,5-difluorophenyl)methyl]amino]phenyl]-1-pentyl- (CA INDEX NAME)

RN 1008763-69-6 ZCAPLUS
CN 1H-Pyrrole-2-carboxylic acid, 4-[4-[[(3,5-difluorophenyl)methyl]amino]phenyl]-1-hexyl- (CA INDEX NAME)

RN 1008763-71-0 ZCAPLUS
CN 1H-Pyrrole-2-carboxylic acid, 4-[4-[[(3,5-difluorophenyl)methyl]amino]phenyl]-1-heptyl- (CA INDEX NAME)

RN 1008763-73-2 ZCAPLUS
CN 1H-Pyrrole-2-carboxylic acid, 4-[4-[[(3,5-difluorophenyl)methyl]amino]phenyl]-1-octyl- (CA INDEX NAME)

RN 1008763-75-4 ZCAPLUS
CN 1H-Pyrrole-2-carboxylic acid, 1-[(3-chlorophenyl)methyl]-4-[4-[[(2,4-difluorophenyl)methyl]amino]phenyl]- (CA INDEX NAME)

PAGE 2-A

RN 1008763-77-6 ZCAPLUS

CN 1H-Pyrrole-2-carboxylic acid, 1-[(4-chlorophenyl)methyl]-4-[4-[(2,4-difluorophenyl)methyl]amino]phenyl]- (CA INDEX NAME)

PAGE 2-A

RN 1008763-79-8 ZCAPLUS

CN 1H-Pyrrole-2-carboxylic acid, 4-[4-[[(2,4-difluorophenyl)methyl]amino]phenyl]-1-hexyl- (CA INDEX NAME)

RN 1008763-81-2 ZCAPLUS CN 1H-Pyrrole-2-carboxylic acid, 4-[4-[[(2,4-difluorophenyl)methyl]amino]phenyl]-1-heptyl- (CA INDEX NAME)

RN 1008763-83-4 ZCAPLUS
CN 1H-Pyrrole-2-carboxylic acid, 4-[4-[[(2,4-difluorophenyl)methyl]amino]phenyl]-1-octyl- (CA INDEX NAME)

RN 1008763-85-6 ZCAPLUS

CN 1H-Pyrrole-2-carboxylic acid, 1-[(3-chlorophenyl)methyl]-4-[4-[[(2,5-difluorophenyl)methyl]amino]phenyl]- (CA INDEX NAME)

PAGE 1-A

RN 1008763-87-8 ZCAPLUS

CN 1H-Pyrrole-2-carboxylic acid, 1-[(4-chlorophenyl)methyl]-4-[4-[[(2,5-difluorophenyl)methyl]amino]phenyl]- (CA INDEX NAME)

PAGE 1-A

PAGE 2-A

RN 1008763-89-0 ZCAPLUS

CN 1H-Pyrrole-2-carboxylic acid, 4-[4-[[(2,5-difluorophenyl)methyl]amino]phenyl]-1-hexyl- (CA INDEX NAME)

RN 1008763-91-4 ZCAPLUS
CN 1H-Pyrrole-2-carboxylic acid, 4-[4-[[(2,5-difluorophenyl)methyl]amino]phenyl]-1-heptyl- (CA INDEX NAME)

RN 1008763-93-6 ZCAPLUS
CN 1H-Pyrrole-2-carboxylic acid, 4-[4-[[(2,5-difluorophenyl)methyl]amino]phenyl]-1-octyl- (CA INDEX NAME)

1008764-56-4P 1008764-58-6P 1008764-61-1P ΙT 1008764-64-4P 1008764-67-7P 1008764-69-9P 1008764-71-3P 1008764-73-5P 1008764-75-7P 1008764-77-9P 1008764-79-1P 1008764-81-5P 1008764-83-7P 1008764-86-0P 1008764-88-2P 1008764-90-6P 1008764-92-8P 1008764-94-0P 1008764-97-3P 1008764-99-5P 1008765-01-2P 1008765-03-4P 1008765-05-6P 1008765-07-8P 1008765-09-0P 1008765-12-5P 1008765-15-8P 1008765-18-1P 1008765-21-6P 1008765-23-8P 1008765-25-0P 1008765-28-3P 1008765-30-7P 1008765-33-0P 1008765-35-2P 1008765-37-4P 1008765-39-6P 1008765-41-0P 1008765-43-2P 1008765-45-4P 1008765-47-6P 1008765-49-8P 1008765-51-2P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(intermediate; preparation of pyrrole derivs. as inhibitors of fatty acid synthase for treating bacterial infection)

RN 1008764-56-4 ZCAPLUS

CN 1H-Pyrrole-2-carboxylic acid, 4-(4-nitrophenyl)-, methyl ester (CA INDEX NAME)

RN 1008764-58-6 ZCAPLUS

CN 1H-Pyrrole-2-carboxylic acid, 1-[(6-chloro-1,3-benzodioxol-5-yl)methyl]-4-(4-nitrophenyl)-, methyl ester (CA INDEX NAME)

RN 1008764-61-1 ZCAPLUS

CN 1H-Pyrrole-2-carboxylic acid, 4-(4-aminophenyl)-1-[(6-chloro-1,3-benzodioxol-5-yl)methyl]-, methyl ester (CA INDEX NAME)

$$\begin{array}{c} \text{O} \\ \text{C-OMe} \\ \\ \text{N-CH}_2 \\ \\ \text{C1} \end{array}$$

RN 1008764-64-4 ZCAPLUS

CN 1H-Pyrrole-2-carboxylic acid, 1-[(6-chloro-1,3-benzodioxol-5-yl)methyl]-4-[4-[[(2,6-dichlorophenyl)methyl]amino]phenyl]-, methyl ester (CA INDEX NAME)

$$\begin{array}{c} \text{C} \\ \text{$$

RN 1008764-67-7 ZCAPLUS

CN 1H-Pyrrole-2-carboxylic acid, 1-[(2-chlorophenyl)methyl]-4-(4-nitrophenyl)-, methyl ester (CA INDEX NAME)

RN 1008764-69-9 ZCAPLUS

CN 1H-Pyrrole-2-carboxylic acid, 4-(4-aminophenyl)-1-[(2-chlorophenyl)methyl]-, methyl ester (CA INDEX NAME)

RN 1008764-71-3 ZCAPLUS

CN 1H-Pyrrole-2-carboxylic acid, 1-[(2-chlorophenyl)methyl]-4-[4-[[(2,6-dichlorophenyl)methyl]amino]phenyl]-, methyl ester (CA INDEX NAME)

RN 1008764-73-5 ZCAPLUS

CN 1H-Pyrrole-2-carboxylic acid, 1-[(3-chlorophenyl)methyl]-4-(4-nitrophenyl)-, methyl ester (CA INDEX NAME)

RN 1008764-75-7 ZCAPLUS

CN 1H-Pyrrole-2-carboxylic acid, 4-(4-aminophenyl)-1-[(3-chlorophenyl)methyl]-, methyl ester (CA INDEX NAME)

$$\begin{array}{c} \text{CH}_2 \\ \text{N} \\ \text{C-OMe} \end{array}$$

RN 1008764-77-9 ZCAPLUS

CN 1H-Pyrrole-2-carboxylic acid, 1-[(3-chlorophenyl)methyl]-4-[4-[[(2,6-dichlorophenyl)methyl]amino]phenyl]-, methyl ester (CA INDEX NAME)

PAGE 1-A

RN 1008764-79-1 ZCAPLUS

CN 1H-Pyrrole-2-carboxylic acid, 1-[(4-chlorophenyl)methyl]-4-(4-nitrophenyl)-, methyl ester (CA INDEX NAME)

RN 1008764-81-5 ZCAPLUS

CN 1H-Pyrrole-2-carboxylic acid, 4-(4-aminophenyl)-1-[(4-chlorophenyl)methyl]-, methyl ester (CA INDEX NAME)

RN 1008764-83-7 ZCAPLUS

CN 1H-Pyrrole-2-carboxylic acid, 1-[(4-chlorophenyl)methyl]-4-[4-[[(2,6-dichlorophenyl)methyl]amino]phenyl]-, methyl ester (CA INDEX NAME)

RN 1008764-86-0 ZCAPLUS

CN 1H-Pyrrole-2-carboxylic acid, 4-(4-nitrophenyl)-1-pentyl-, methyl ester (CA INDEX NAME)

RN 1008764-88-2 ZCAPLUS

CN 1H-Pyrrole-2-carboxylic acid, 4-(4-aminophenyl)-1-pentyl-, methyl ester (CA INDEX NAME)

RN 1008764-90-6 ZCAPLUS

CN 1H-Pyrrole-2-carboxylic acid, 4-[4-[[(2,6-dichlorophenyl)methyl]amino]phenyl]-1-pentyl-, methyl ester (CA INDEX NAME)

RN 1008764-92-8 ZCAPLUS

CN 1H-Pyrrole-2-carboxylic acid, 1-hexyl-4-(4-nitrophenyl)-, methyl ester (CA INDEX NAME)

RN 1008764-94-0 ZCAPLUS

CN 1H-Pyrrole-2-carboxylic acid, 4-(4-aminophenyl)-1-hexyl-, methyl ester

(CA INDEX NAME)

RN 1008764-97-3 ZCAPLUS

CN 1H-Pyrrole-2-carboxylic acid, 4-[4-[[(2,6-dichlorophenyl)methyl]amino]phenyl]-1-hexyl-, methyl ester (CA INDEX NAME)

RN 1008764-99-5 ZCAPLUS

CN 1H-Pyrrole-2-carboxylic acid, 1-heptyl-4-(4-nitrophenyl)-, methyl ester (CA INDEX NAME)

RN 1008765-01-2 ZCAPLUS

CN 1H-Pyrrole-2-carboxylic acid, 4-(4-aminophenyl)-1-heptyl-, methyl ester (CA INDEX NAME)

RN 1008765-03-4 ZCAPLUS

CN 1H-Pyrrole-2-carboxylic acid, 4-[4-[[(2,6-dichlorophenyl)methyl]amino]phenyl]-1-heptyl-, methyl ester (CA INDEX NAME)

RN 1008765-05-6 ZCAPLUS

CN 1H-Pyrrole-2-carboxylic acid, 4-(4-nitrophenyl)-1-octyl-, methyl ester (CA INDEX NAME)

RN 1008765-07-8 ZCAPLUS

CN 1H-Pyrrole-2-carboxylic acid, 4-(4-aminophenyl)-1-octyl-, methyl ester (CA INDEX NAME)

RN 1008765-09-0 ZCAPLUS

CN 1H-Pyrrole-2-carboxylic acid, 4-[4-[[(2,6-dichlorophenyl)methyl]amino]phenyl]-1-octyl-, methyl ester (CA INDEX NAME)

RN 1008765-12-5 ZCAPLUS

 $\texttt{CN} \qquad 1 \\ \texttt{H-Pyrrole-2-carboxylic acid, 1-[(6-chloro-1,3-benzodioxol-5-yl)methyl]-4-leading of the property of the prope$ 

[4-[[(3,5-difluorophenyl)methyl]amino]phenyl]-, methyl ester (CA INDEX NAME)

$$\begin{array}{c} \text{C} \\ \text{$$

RN 1008765-15-8 ZCAPLUS

CN 1H-Pyrrole-2-carboxylic acid, 1-[(2-chlorophenyl)methyl]-4-[4-[[(3,5-difluorophenyl)methyl]amino]phenyl]-, methyl ester (CA INDEX NAME)

PAGE 1-A

PAGE 2-A

RN 1008765-18-1 ZCAPLUS

CN 1H-Pyrrole-2-carboxylic acid, 1-[(3-chlorophenyl)methyl]-4-[4-[[(3,5-difluorophenyl)methyl]amino]phenyl]-, methyl ester (CA INDEX NAME)

PAGE 2-A

RN 1008765-21-6 ZCAPLUS

CN 1H-Pyrrole-2-carboxylic acid, 1-[(4-chlorophenyl)methyl]-4-[4-[[(3,5-difluorophenyl)methyl]amino]phenyl]-, methyl ester (CA INDEX NAME)

PAGE 2-A

RN 1008765-23-8 ZCAPLUS

CN 1H-Pyrrole-2-carboxylic acid, 4-[4-[[(3,5-difluorophenyl)methyl]amino]phenyl]-1-pentyl-, methyl ester (CA INDEX NAME)

RN 1008765-25-0 ZCAPLUS

CN 1H-Pyrrole-2-carboxylic acid, 4-[4-[[(3,5-difluorophenyl)methyl]amino]phenyl]-1-hexyl-, methyl ester (CA INDEX NAME)

RN 1008765-28-3 ZCAPLUS

CN 1H-Pyrrole-2-carboxylic acid, 4-[4-[[(3,5-difluorophenyl)methyl]amino]phenyl]-1-heptyl-, methyl ester (CA INDEX NAME)

RN 1008765-30-7 ZCAPLUS

CN 1H-Pyrrole-2-carboxylic acid, 4-[4-[[(3,5-difluorophenyl)methyl]amino]phenyl]-1-octyl-, methyl ester (CA INDEX NAME)

RN 1008765-33-0 ZCAPLUS

CN 1H-Pyrrole-2-carboxylic acid, 1-[(3-chlorophenyl)methyl]-4-[4-[[(2,4-difluorophenyl)methyl]amino]phenyl]-, methyl ester (CA INDEX NAME)

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RN 1008765-35-2 ZCAPLUS

CN 1H-Pyrrole-2-carboxylic acid, 1-[(4-chlorophenyl)methyl]-4-[4-[[(2,4-difluorophenyl)methyl]amino]phenyl]-, methyl ester (CA INDEX NAME)

RN 1008765-37-4 ZCAPLUS

CN 1H-Pyrrole-2-carboxylic acid, 4-[4-[[(2,4-difluorophenyl)methyl]amino]phenyl]-1-hexyl-, methyl ester (CA INDEX NAME)

RN 1008765-39-6 ZCAPLUS

CN 1H-Pyrrole-2-carboxylic acid, 4-[4-[[(2,4-difluorophenyl)methyl]amino]phenyl]-1-heptyl-, methyl ester (CA INDEX NAME)

RN 1008765-41-0 ZCAPLUS

CN 1H-Pyrrole-2-carboxylic acid, 4-[4-[[(2,4-difluorophenyl)methyl]amino]phenyl]-1-octyl-, methyl ester (CA INDEX NAME)

RN

1008765-43-2 ZCAPLUS
1H-Pyrrole-2-carboxylic acid, 1-[(3-chlorophenyl)methyl]-4-[4-[[(2,5-difluorophenyl)methyl]amino]phenyl]-, methyl ester (CA INDEX NAME) CN

PAGE 1-A

- RN 1008765-45-4 ZCAPLUS
- CN 1H-Pyrrole-2-carboxylic acid, 1-[(4-chlorophenyl)methyl]-4-[4-[[(2,5-difluorophenyl)methyl]amino]phenyl]-, methyl ester (CA INDEX NAME)

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- RN 1008765-47-6 ZCAPLUS
- CN 1H-Pyrrole-2-carboxylic acid, 4-[4-[[(2,5-difluorophenyl)methyl]amino]phenyl]-1-hexyl-, methyl ester (CA INDEX NAME)

RN 1008765-49-8 ZCAPLUS

CN 1H-Pyrrole-2-carboxylic acid, 4-[4-[[(2,5-difluorophenyl)methyl]amino]phenyl]-1-heptyl-, methyl ester (CA INDEX NAME)

RN 1008765-51-2 ZCAPLUS

CN 1H-Pyrrole-2-carboxylic acid, 4-[4-[[(2,5-difluorophenyl)methyl]amino]phenyl]-1-octyl-, methyl ester (CA INDEX NAME)

L32 ANSWER 4 OF 14 ZCAPLUS COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 2005:99322 ZCAPLUS

DOCUMENT NUMBER: 142:172178

TITLE: Pyrrole-based receptor tyrosine kinase inhibitors for

use in disease treatment

INVENTOR(S): Kim, Annette S.

PATENT ASSIGNEE(S): Merck & Co., Inc., USA SOURCE: PCT Int. Appl., 58 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND DATE	APPLICATION NO.	DATE
WO 2005009373 WO 2005009373	A2 20050203 A3 20050909		20040720
W: AE, AG, A CN, CO, C GE, GH, G LK, LR, L NO, NZ, O TJ, TM, T RW: BW, GH, G AZ, BY, K EE, ES, F	L, AM, AT, AU, AZ, R, CU, CZ, DE, DK, M, HR, HU, ID, IL, S, LT, LU, LV, MA, M, PG, PH, PL, PT, N, TR, TT, TZ, UA, M, KE, LS, MW, MZ, G, KZ, MD, RU, TJ, I, FR, GB, GR, HU, R, BF, BJ, CF, CG,	BA, BB, BG, BR, BW, BY, DM, DZ, EC, EE, EG, ES, IN, IS, JP, KE, KG, KP, MD, MG, MK, MN, MW, MX, RO, RU, SC, SD, SE, SG, UG, US, UZ, VC, VN, YU, NA, SD, SL, SZ, TZ, UG, TM, AT, BE, BG, CH, CY, IE, IT, LU, MC, NL, PL, CI, CM, GA, GN, GQ, GW,	FI, GB, GD, KR, KZ, LC, MZ, NA, NI, SK, SL, SY, ZA, ZM, ZW ZM, ZW, AM, CZ, DE, DK, PI, RO, SE,
AU 2004258963	A1 20050203 A1 20050203		20040720
R: AT, BE, C	H, DE, DK, ES, FR, I, LV, FI, RO, CY, A 20060906 T 20061221	GB, GR, IT, LI, LU, NL, TR, BG, CZ, EE, HU, PL, CN 2004-80021448  JP 2006-521205	SE, MC, PT, SK 20040720 20040720
US 7538231 IN 2006DN00759	B2 20090526 A 20070824		20060215

PRIORITY APPLN. INFO.: US 2003-489699P P 20030724 WO 2004-US23425 W 20040720

OTHER SOURCE(S): CASREACT 142:172178; MARPAT 142:172178

IT 832132-57-7P

RL: SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(pyrrole-based receptor tyrosine kinase inhibitors for use in disease treatment)

RN 832132-57-7 ZCAPLUS

CN 1H-Pyrrole-2-carboxylic acid, 3-ethyl-5-formyl-4-(4-nitrophenyl)-, 1,1-dimethylethyl ester (CA INDEX NAME)

REFERENCE COUNT: 1 THERE ARE 1 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

=> d his

L1

L18

(FILE 'HOME' ENTERED AT 15:46:59 ON 17 JUN 2009)

FILE 'ZCAPLUS' ENTERED AT 15:50:55 ON 17 JUN 2009

E US2006-591140/APPS E US2007-591140/APPS 1 S US2007-591140/APPS

SEL RN

FILE 'REGISTRY' ENTERED AT 15:53:12 ON 17 JUN 2009

L2 83 S E1-E83 L3 STRUCTURE UPLOADED T. 4 7 S SAM SSS L3 STRUCTURE UPLOADED L511 S SAM SSS L5 1.6 STRUCTURE UPLOADED L7 0 S SAM SSS L7 L8 STRUCTURE UPLOADED L9 0 S SAM SSS L9 L10

L11 STRUCTURE UPLOADED
L12 11 S SAM SSS L11

L13 STRUCTURE UPLOADED
L14 1 S SAM SSS L13
L15 STRUCTURE UPLOADED

L16 1 S SAM SSS L15

FILE 'ZCAPLUS' ENTERED AT 16:13:46 ON 17 JUN 2009 L17 199018 S POLYAMIDE

FILE 'REGISTRY' ENTERED AT 16:14:05 ON 17 JUN 2009 185 S FULL SSS L11

L19	'ZCAPLUS' ENTERED AT 16:40:06 ON 17 JUN 2009 64 S L18 0 S L19 AND (POLYAMIDE OR POLYAMIDO) 0 S L19 (W) (POLYAMIDE OR POLYAMIDO)		
L22	'REGISTRY' ENTERED AT 16:42:41 ON 17 JUN 2009 1 S L18 SAM SUB=L14 16 S L14 FULL SUB=L18		
L24 L25	'ZCAPLUS' ENTERED AT 16:47:08 ON 17 JUN 2009 8 S L23 0 S L24 AND ?POLYAMID? 1 S L1 SAM SUB=L18		
L27 L28	'REGISTRY' ENTERED AT 17:18:36 ON 17 JUN 2009 0 S L1 SAM SUB=L18 7 S L3 SAM SUB=L18 97 S L3 FULL SUB=L18		
L30 L31 L32	'ZCAPLUS' ENTERED AT 17:23:06 ON 17 JUN 2009 17 S L29 0 S L30 AND ?POLYAMID? 14 S L30 NOT L24 10 S L32 NOT NO2		
	'REGISTRY' ENTERED AT 17:29:28 ON 17 JUN 2009 1 S L29 NOT CAPLUS/LC		
FILE	'ZCAPLUS' ENTERED AT 17:30:03 ON 17 JUN 2009		
LOGOFF? (	ERIES AND ANSWER SETS ARE DELETED AT LOGOFF Y)/N/HOLD:y		
	SINCE FILE TOTAL ENTRY SESSION		
FULL ESTIMATED COST 15.91 449.96			

STN INTERNATIONAL LOGOFF AT 17:32:55 ON 17 JUN 2009